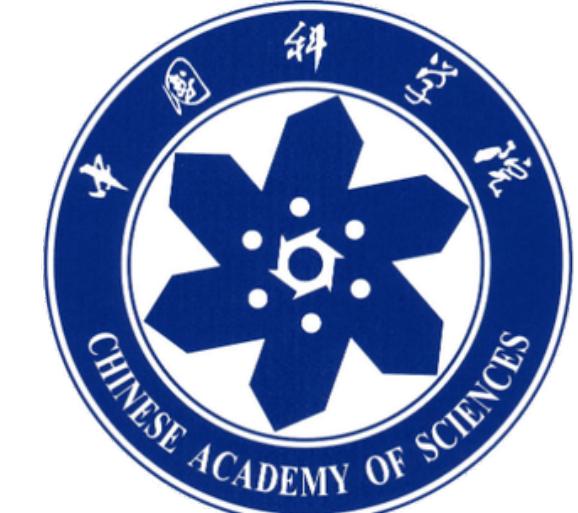
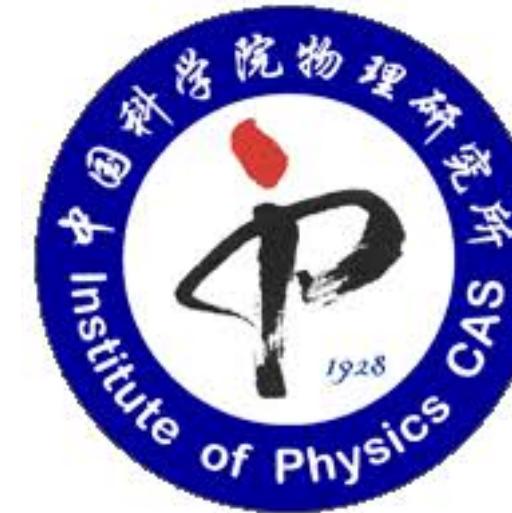


# 流模型：计算物理视角

王磊 中科院物理研究所

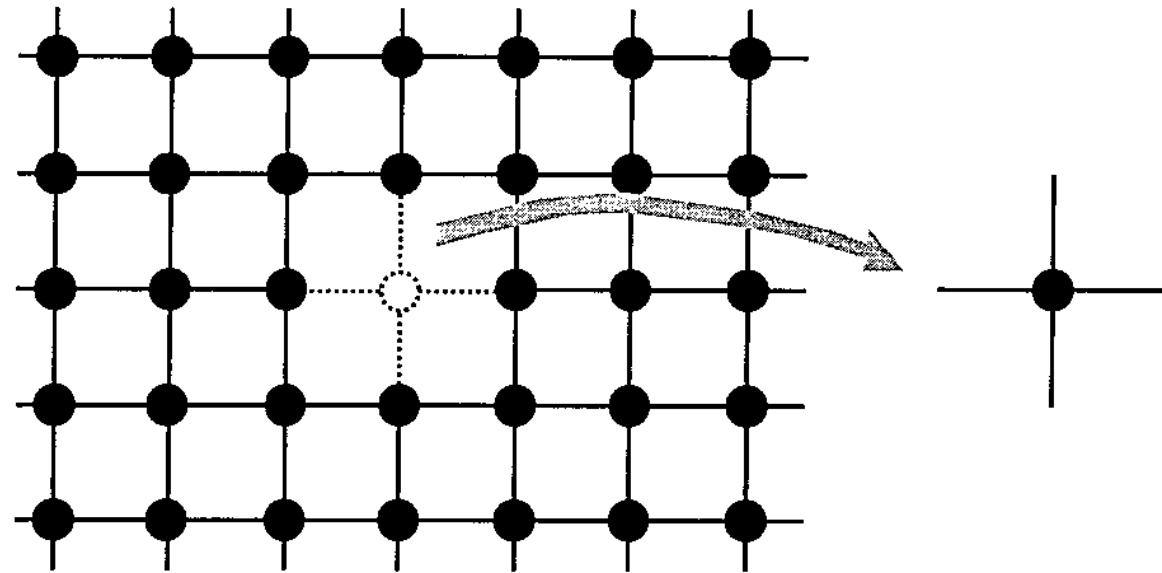
wanglei@iphy.ac.cn

<https://wangleiphy.github.io>

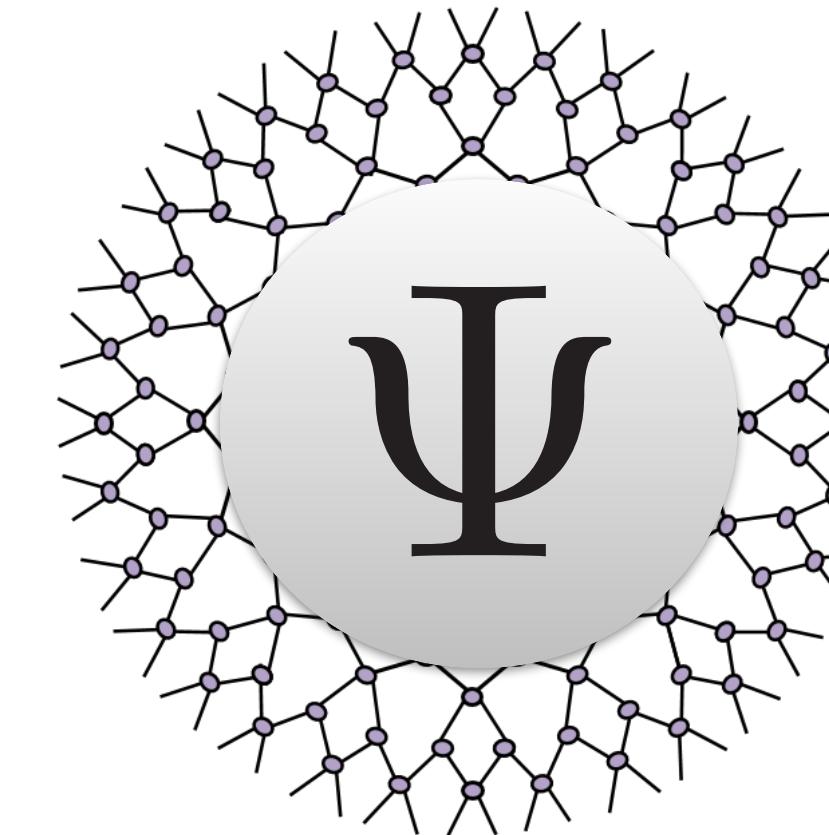


# Physicists' gifts to Machine Learning

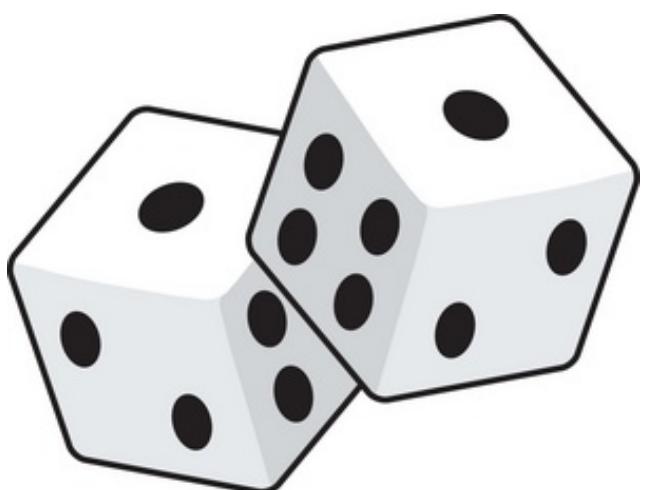
## Mean Field Theory



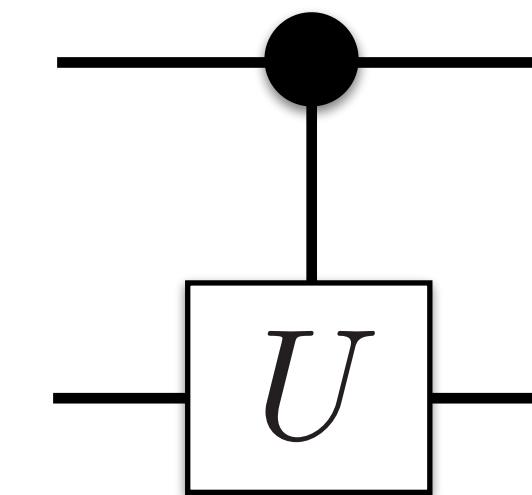
## Tensor Networks



## Monte Carlo Methods



## Quantum Computing



# Deep learning is more than fitting functions



**Discriminative learning**

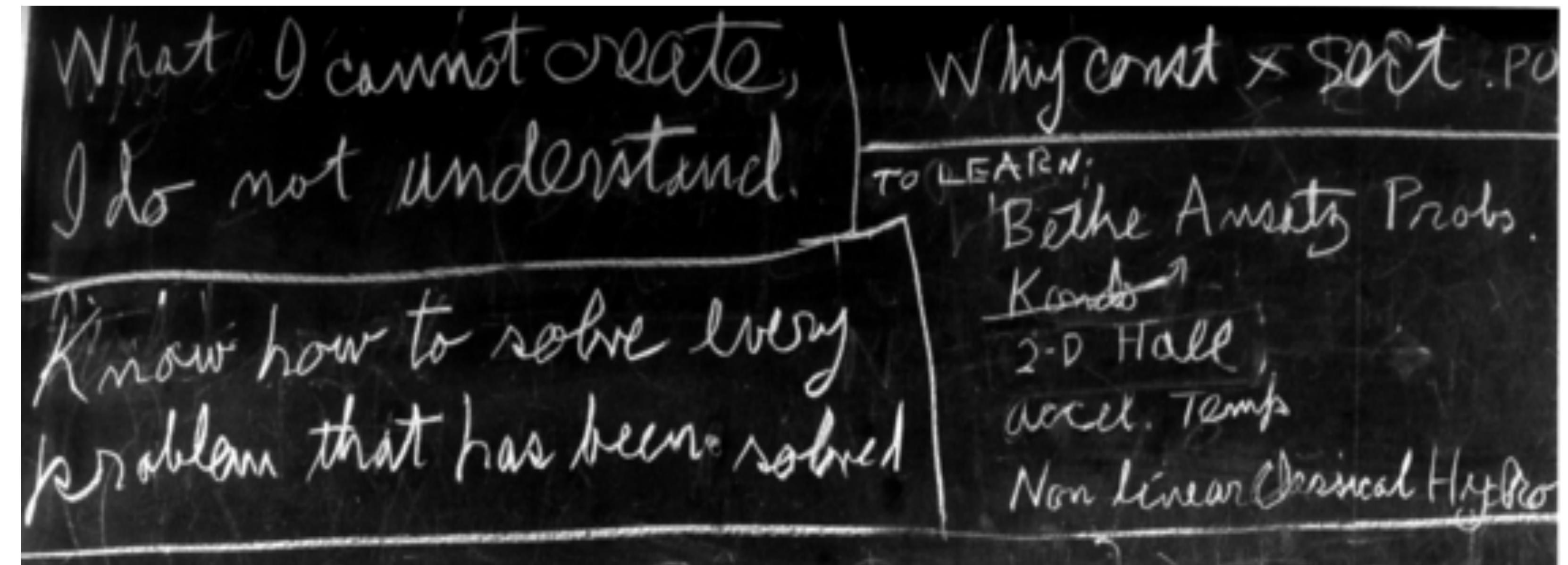
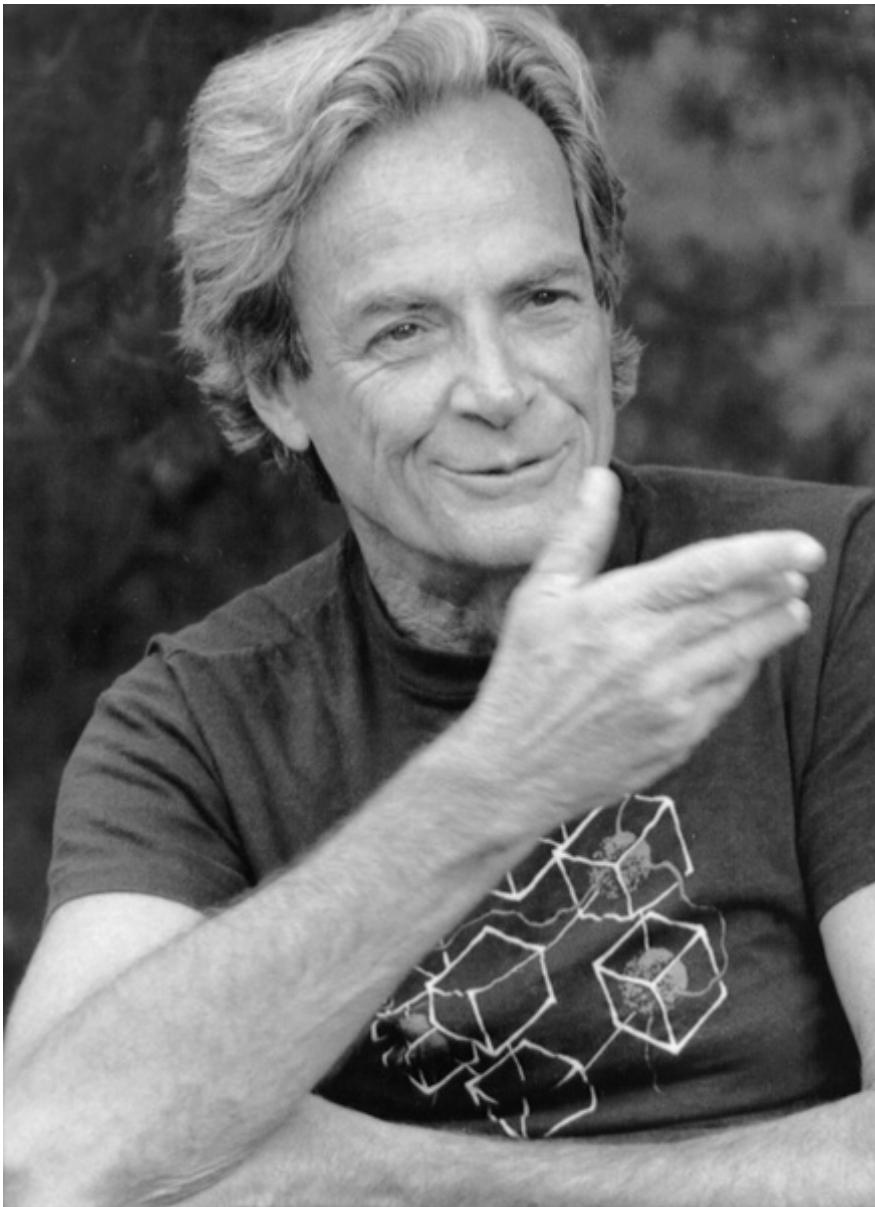
$$y = f(x)$$

or  $p(y | x)$

**Generative learning**

$$p(x, y)$$

# Deep learning is more than fitting functions



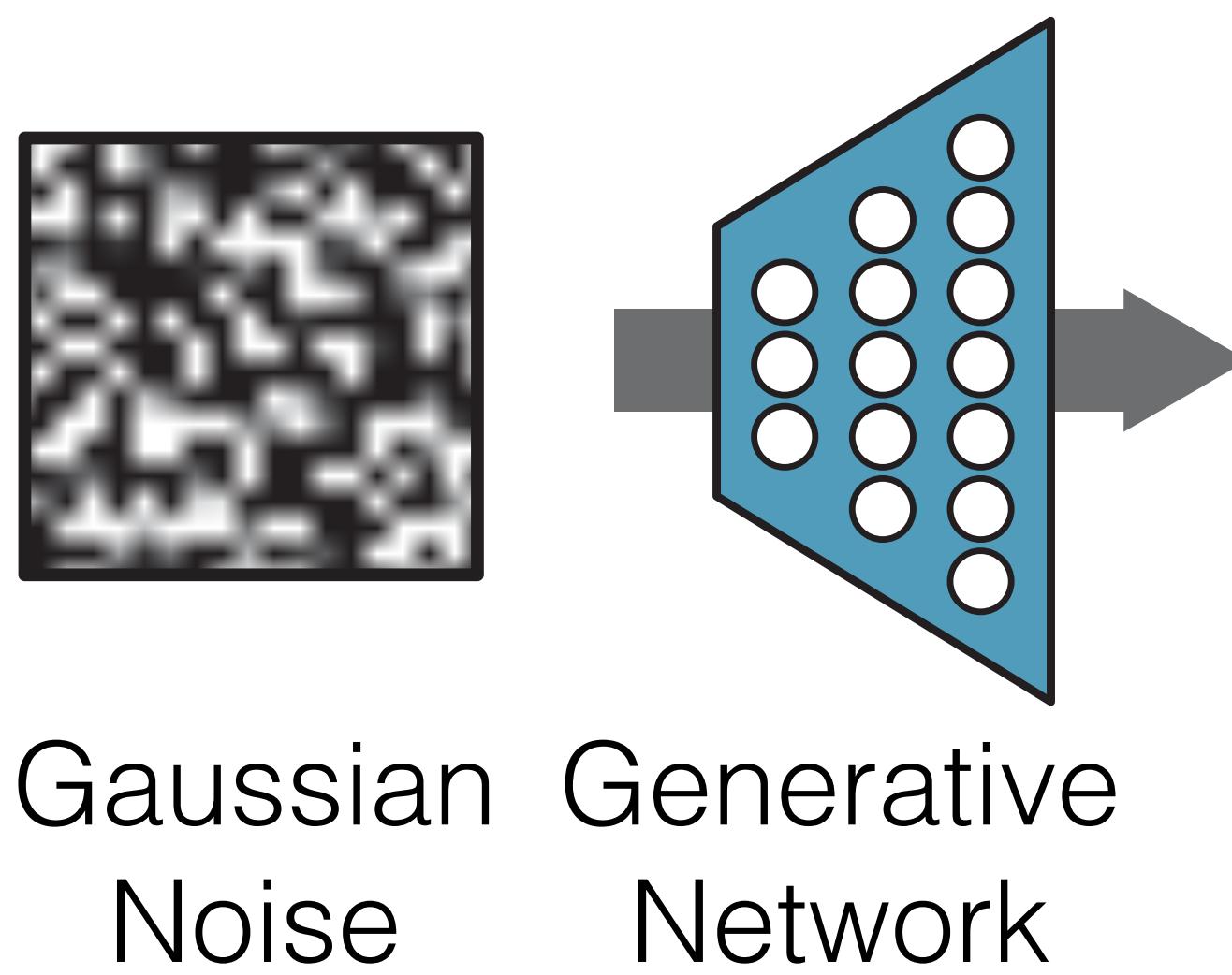
“What I can not create, I do not understand”

# Generated Arts

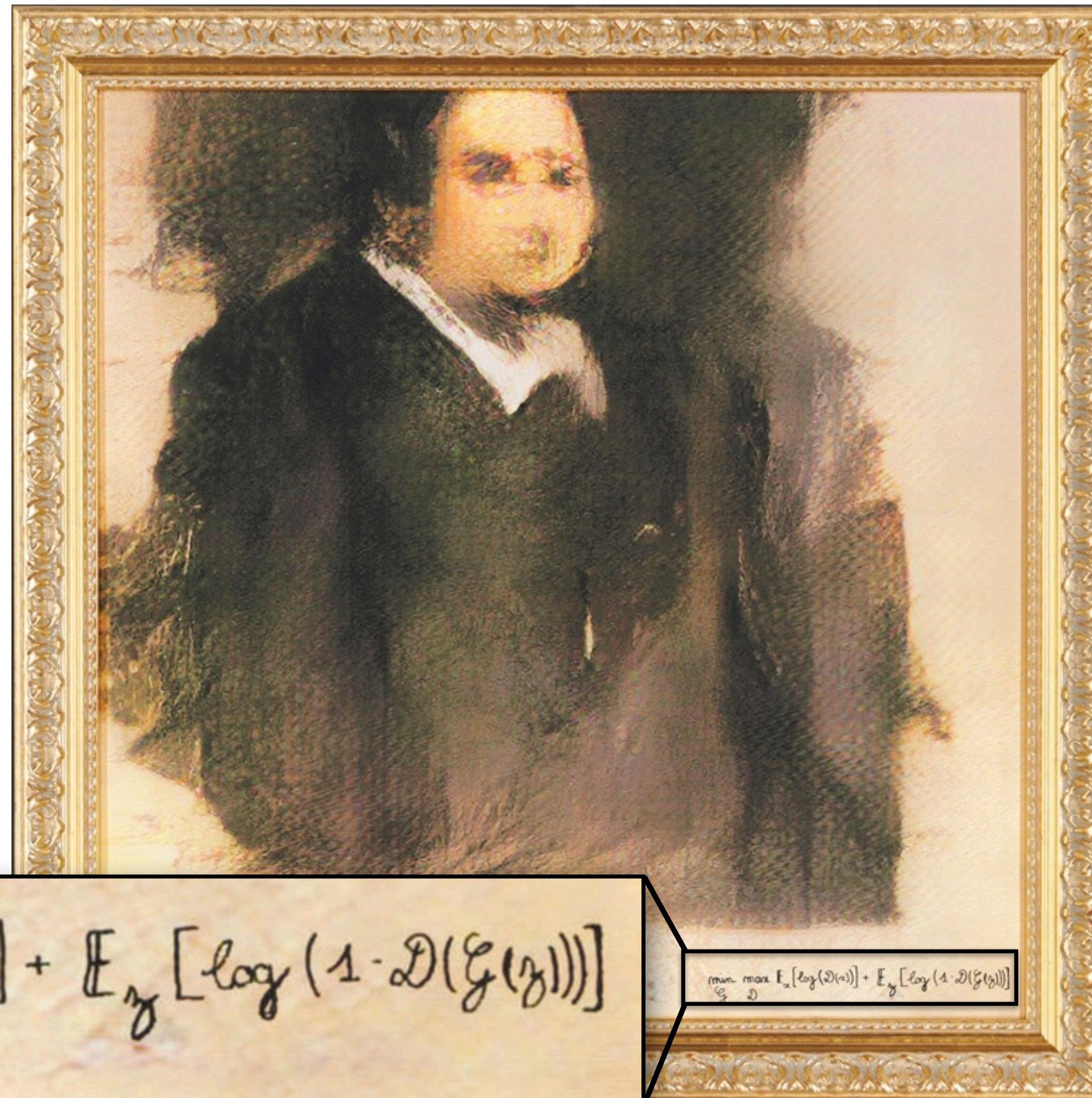


**\$432,500**  
**25 October 2018**  
**Christie's New York**

# Generated Arts



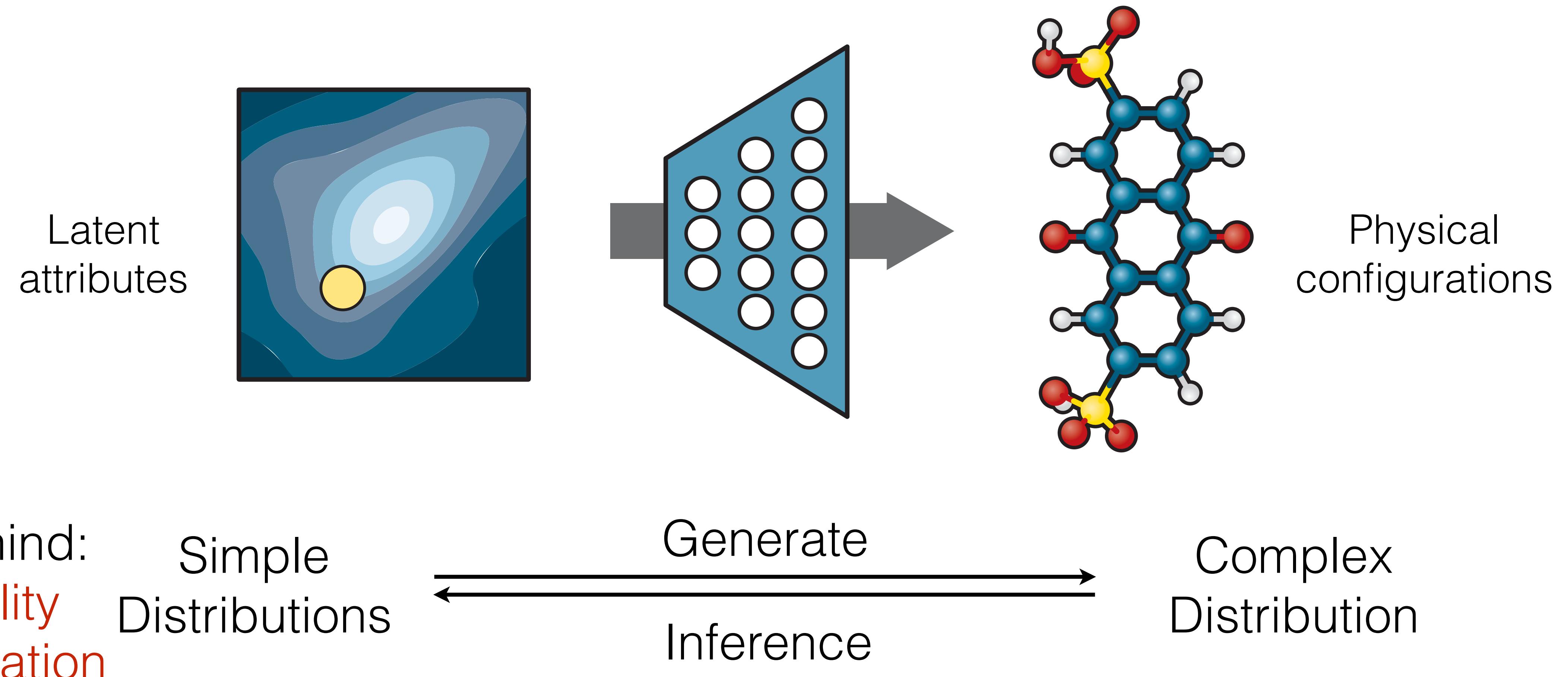
Gaussian Noise      Generative Network



$$\min_{\mathcal{G}} \max_{\mathcal{D}} \mathbb{E}_{\mathbf{x}} [\log(\mathcal{D}(\mathbf{x}))] + \mathbb{E}_{\mathbf{z}} [\log(1 - \mathcal{D}(\mathcal{G}(\mathbf{z})))]$$

\$432,500  
25 October 2018  
Christie's New York

# Generating molecules

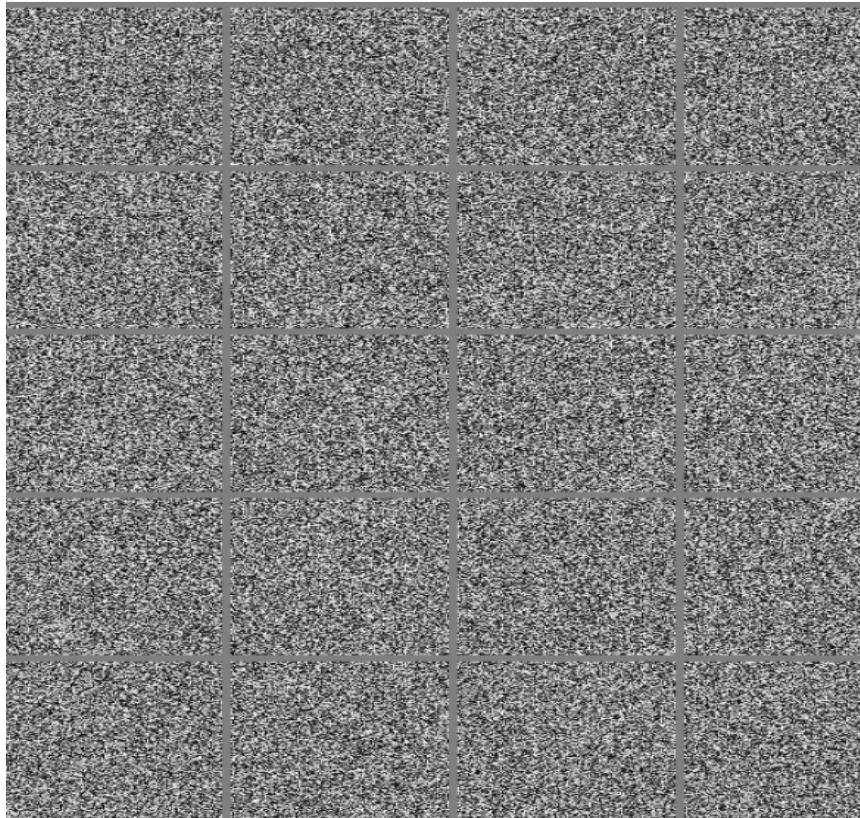


Sanchez-Lengeling & Aspuru-Guzik,  
Inverse molecular design using machine learning:  
Generative models for matter engineering, Science '18

# Probabilistic Generative Modeling

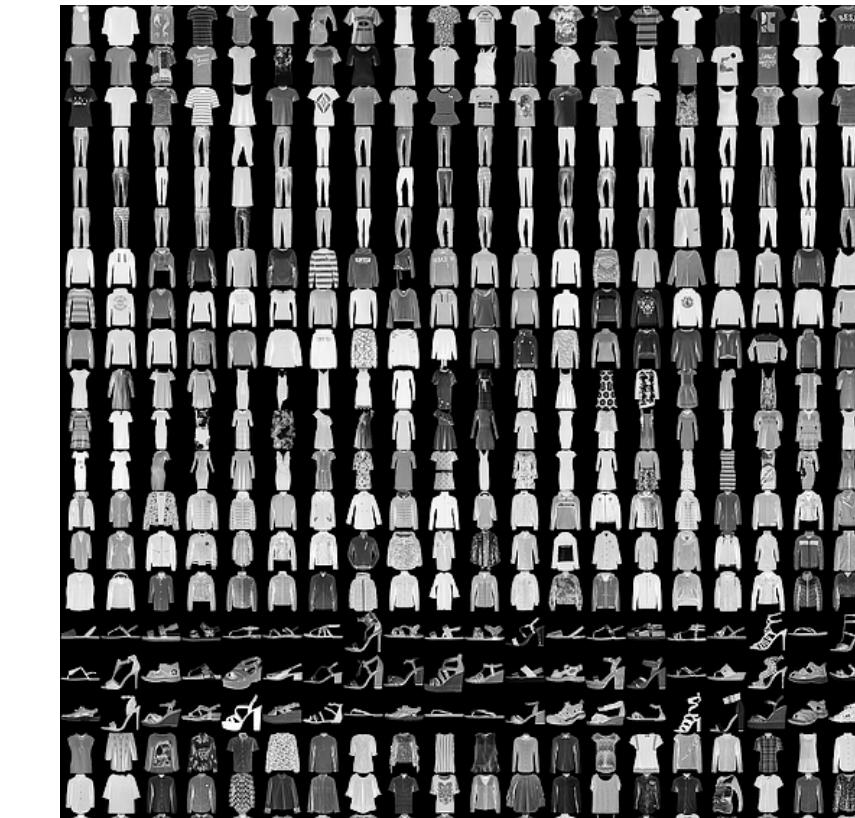
$$p(x)$$

How to express, learn, and sample from a high-dimensional probability distribution ?



“random” images

8	9	0	1	2	3	4	7	8	9	0	1	2	3	4	5	6	7	8	6
4	2	6	4	7	5	5	4	7	8	9	2	9	3	9	3	8	2	0	5
0	1	0	4	2	6	5	3	5	3	8	0	0	3	4	1	5	3	0	8
3	0	6	2	7	1	1	8	1	7	1	3	8	9	7	6	7	4	1	6
7	5	1	7	1	9	8	0	6	9	4	9	9	3	7	1	9	2	2	5
3	7	8	2	3	4	5	6	7	8	9	0	1	2	3	4	5	6	7	0
1	2	3	4	5	6	7	8	9	8	1	0	5	5	1	9	0	4	1	9
3	8	4	7	7	8	5	0	6	5	5	3	3	3	9	8	1	4	0	6
1	0	0	6	2	1	1	3	2	8	8	7	8	4	6	0	2	0	3	6
8	7	1	5	9	9	3	2	4	9	4	4	5	3	2	8	5	9	4	1
6	5	0	1	2	3	4	5	6	7	8	9	0	1	2	3	4	5	6	7
8	9	0	1	2	3	4	5	6	7	8	9	6	4	2	6	4	7	5	5
4	7	8	9	2	9	3	9	3	8	2	0	9	8	0	5	6	0	1	0
4	2	6	5	5	5	4	3	4	1	5	3	0	8	3	0	6	2	7	1
1	8	1	7	1	3	8	5	4	2	0	9	7	6	7	4	1	6	8	4
7	5	1	2	6	7	1	9	8	0	6	9	4	9	9	6	2	3	7	1
9	2	2	5	3	7	8	0	1	2	3	4	5	6	7	8	0	1	2	3
4	5	6	7	8	0	1	2	3	4	5	6	7	8	9	2	1	2	1	3
9	9	8	5	3	7	0	7	7	5	7	9	9	4	7	0	3	4	1	4
4	7	5	8	1	4	8	4	1	8	6	4	6	3	5	7	2	5	9	



“natural” images

# Probabilistic modeling

How to  
high-d

## DEEP LEARNING

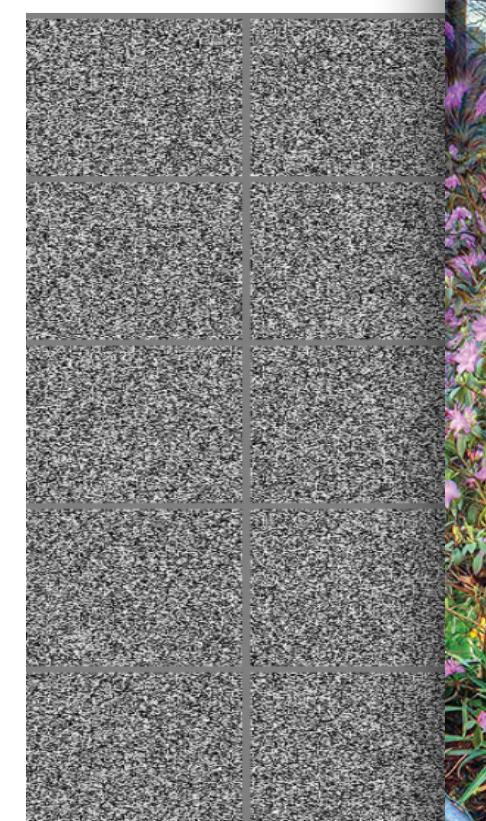
Ian Goodfellow, Yoshua Bengio,  
and Aaron Courville

from a  
solution ?

Page 159

*“... the images encountered in  
AI applications occupy a  
negligible proportion of  
the volume of image space.”*

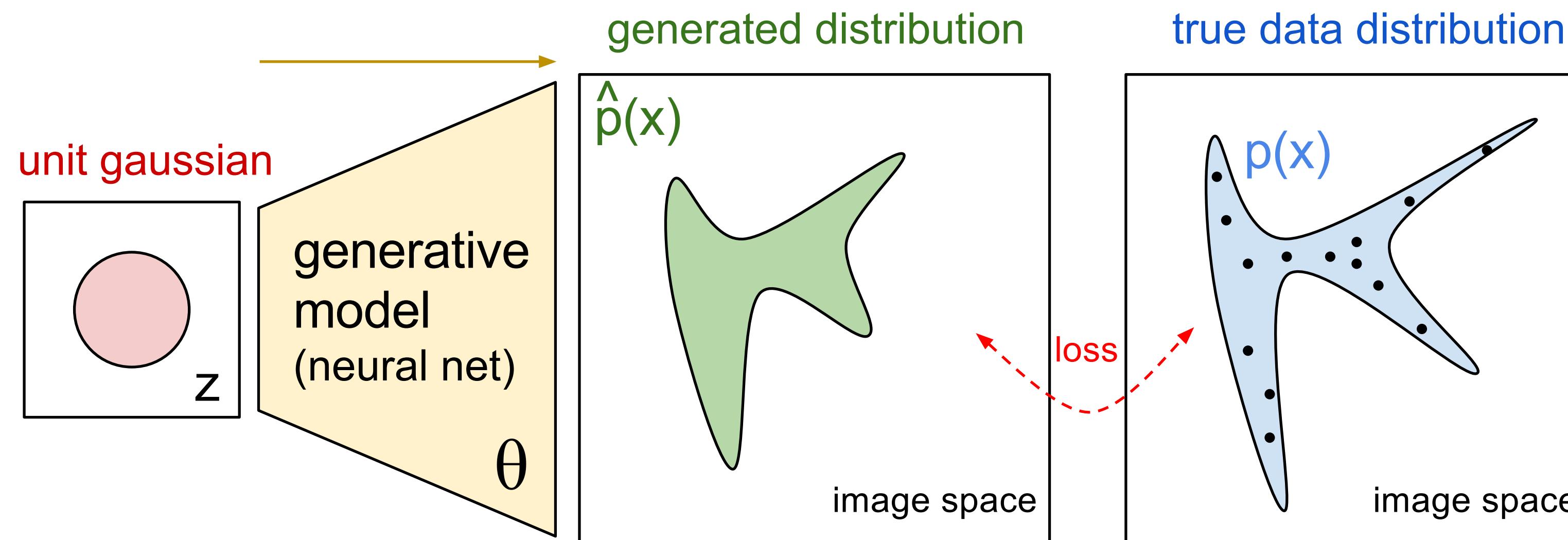
“random”



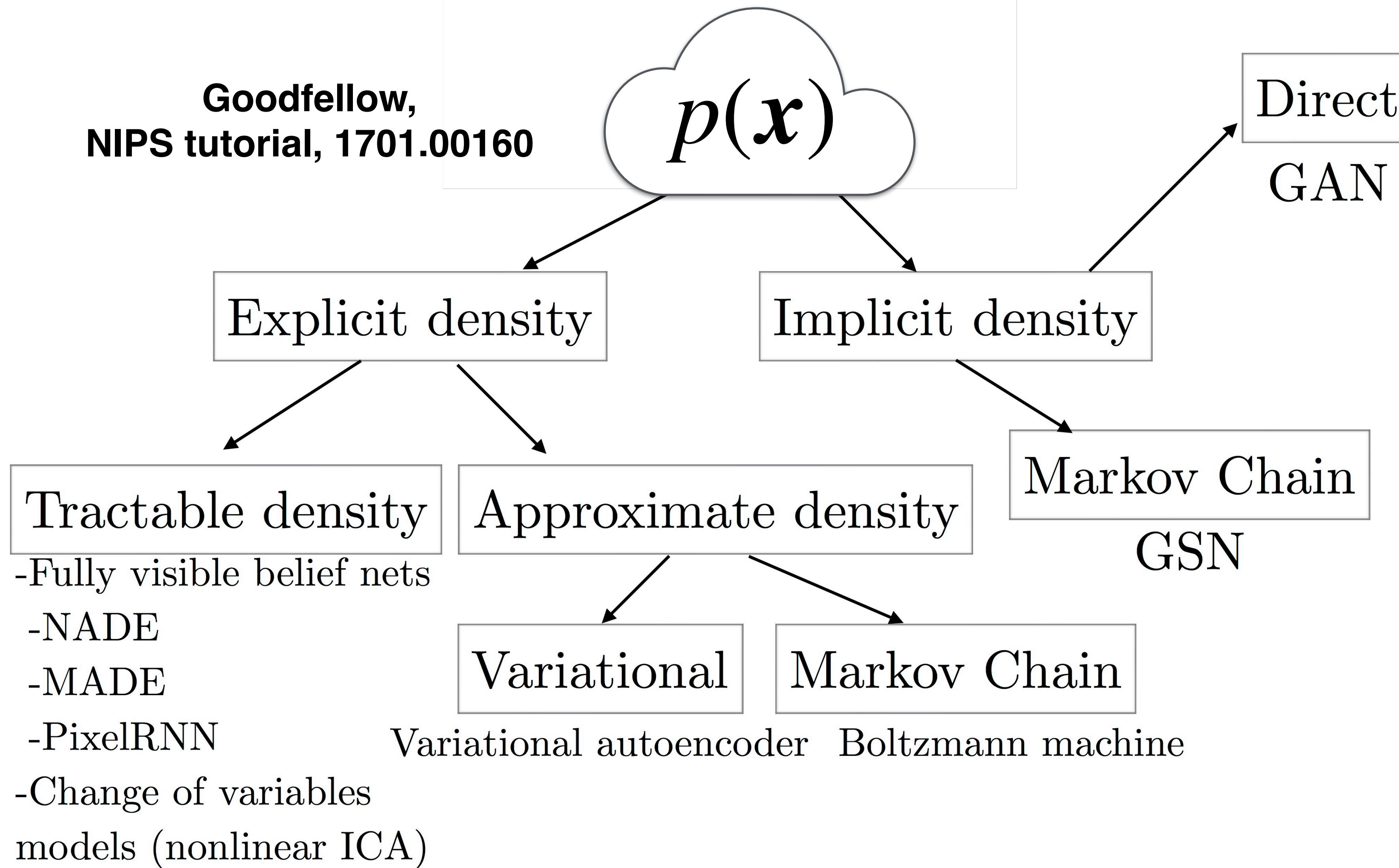
# Probabilistic Generative Modeling

$$p(x)$$

How to express, learn, and sample from a high-dimensional probability distribution ?



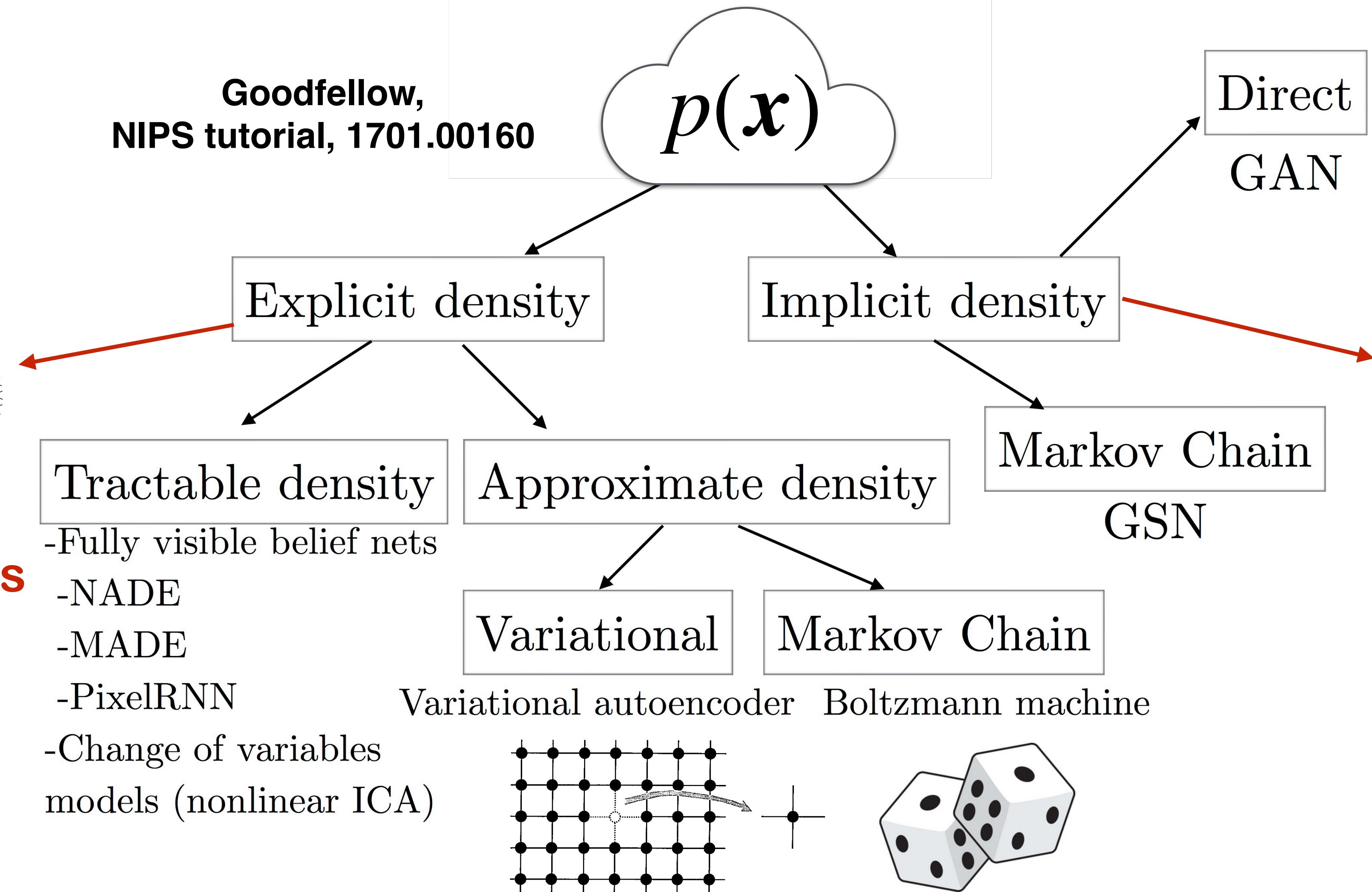
# Physics genes of generative models



# Physics genes of generative models

**Tensor Networks**

Goodfellow,  
NIPS tutorial, 1701.00160

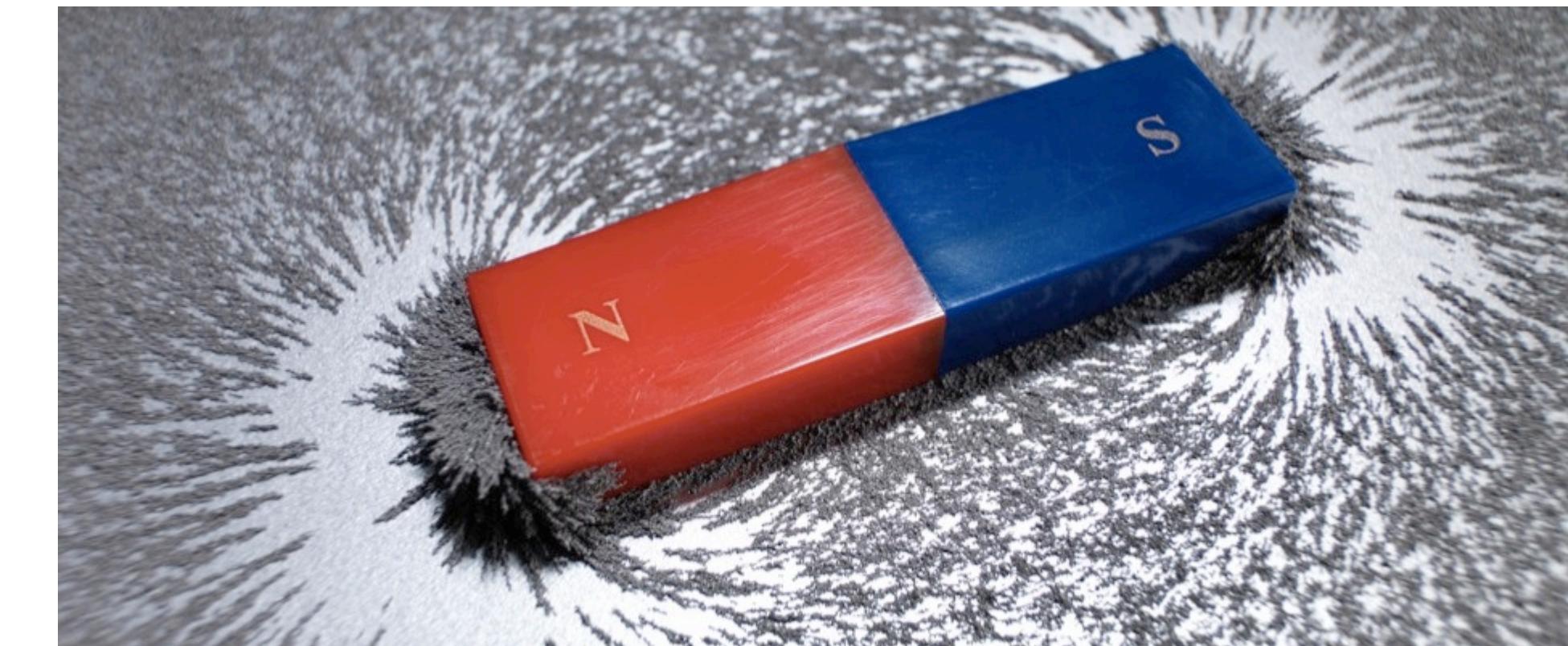


# Generative modeling



Known: samples  
Unknown: generating distribution

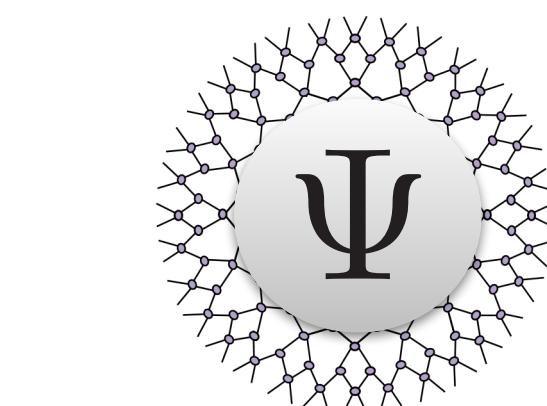
# Physics



Known: energy function  
Unknown: samples, partition function

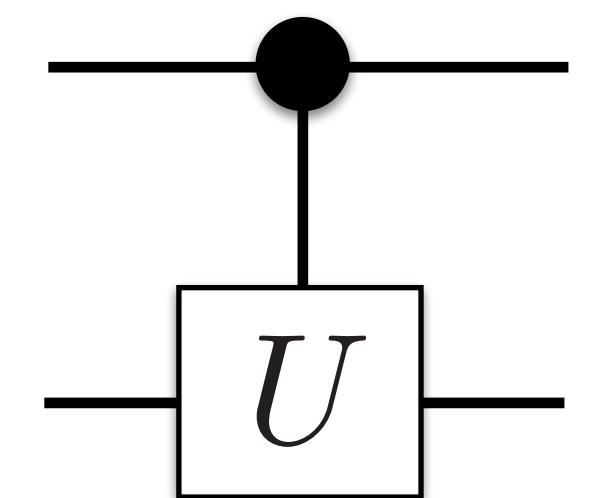
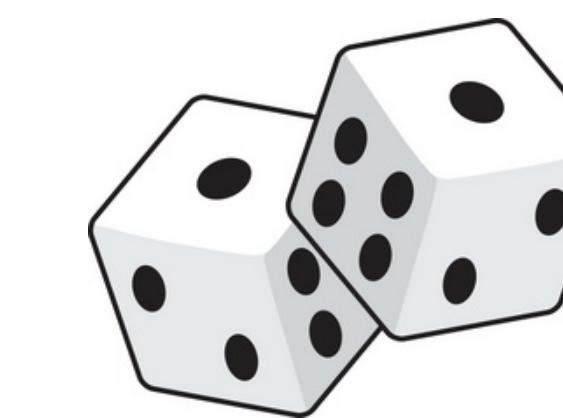
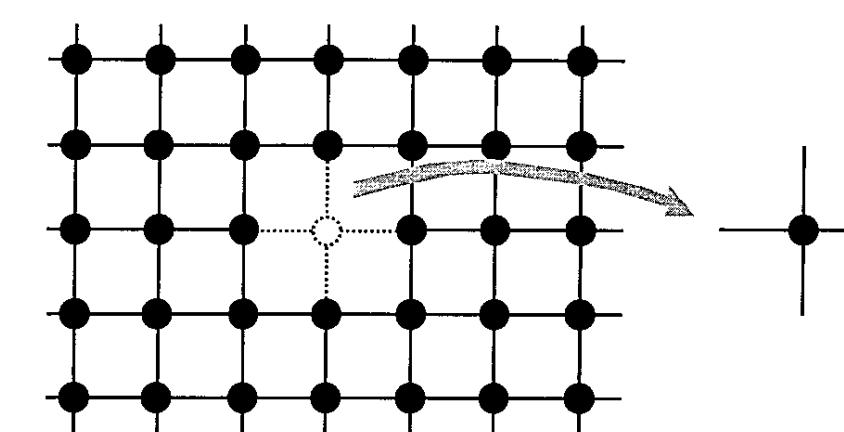
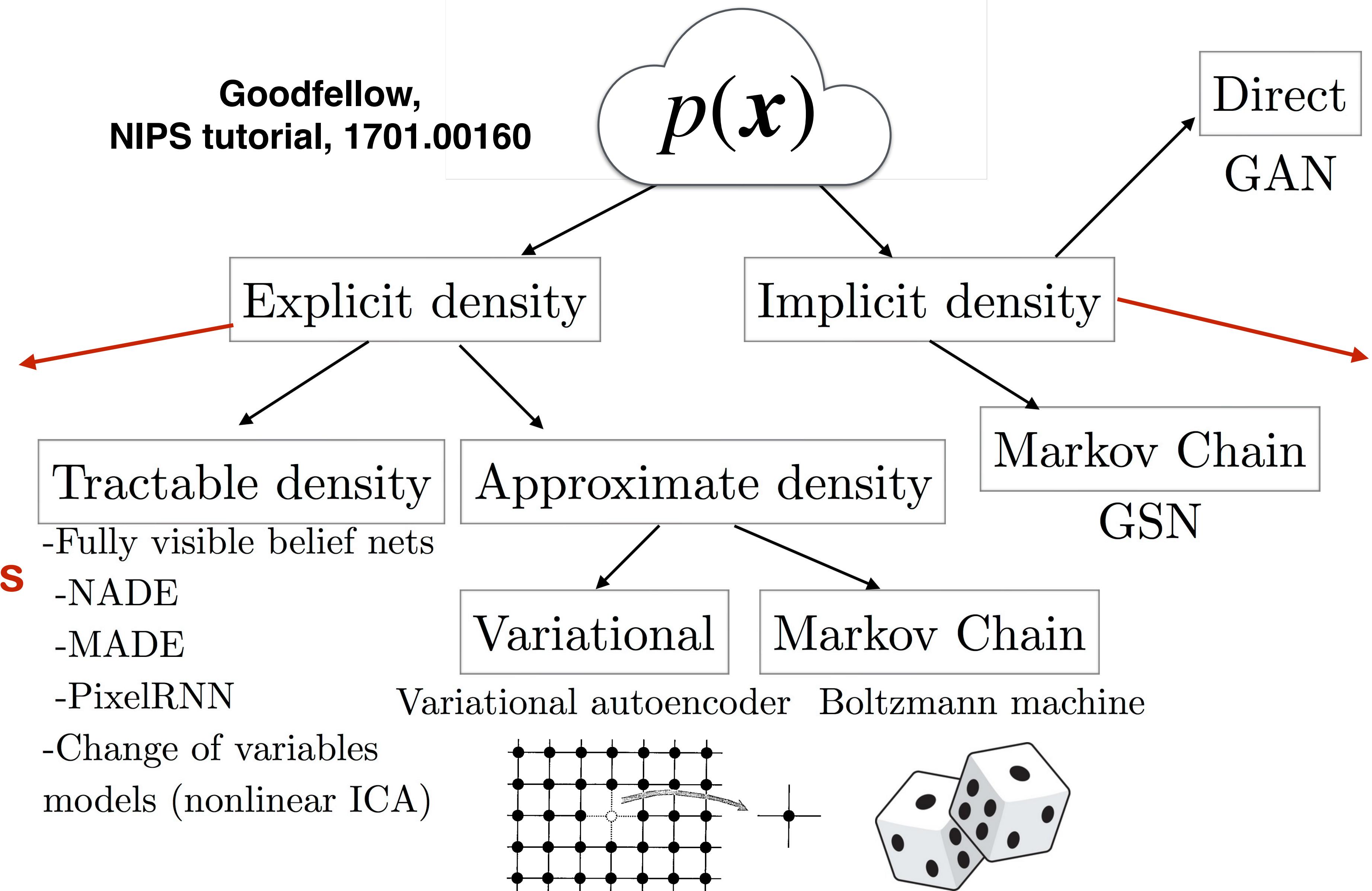
**Modern generative models for physics  
Physics of and for generative modeling**

# Physics genes of generative models



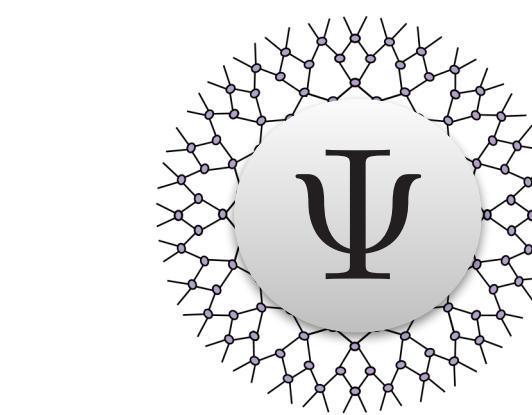
## Tensor Networks

Goodfellow,  
NIPS tutorial, 1701.00160



## Quantum Circuits

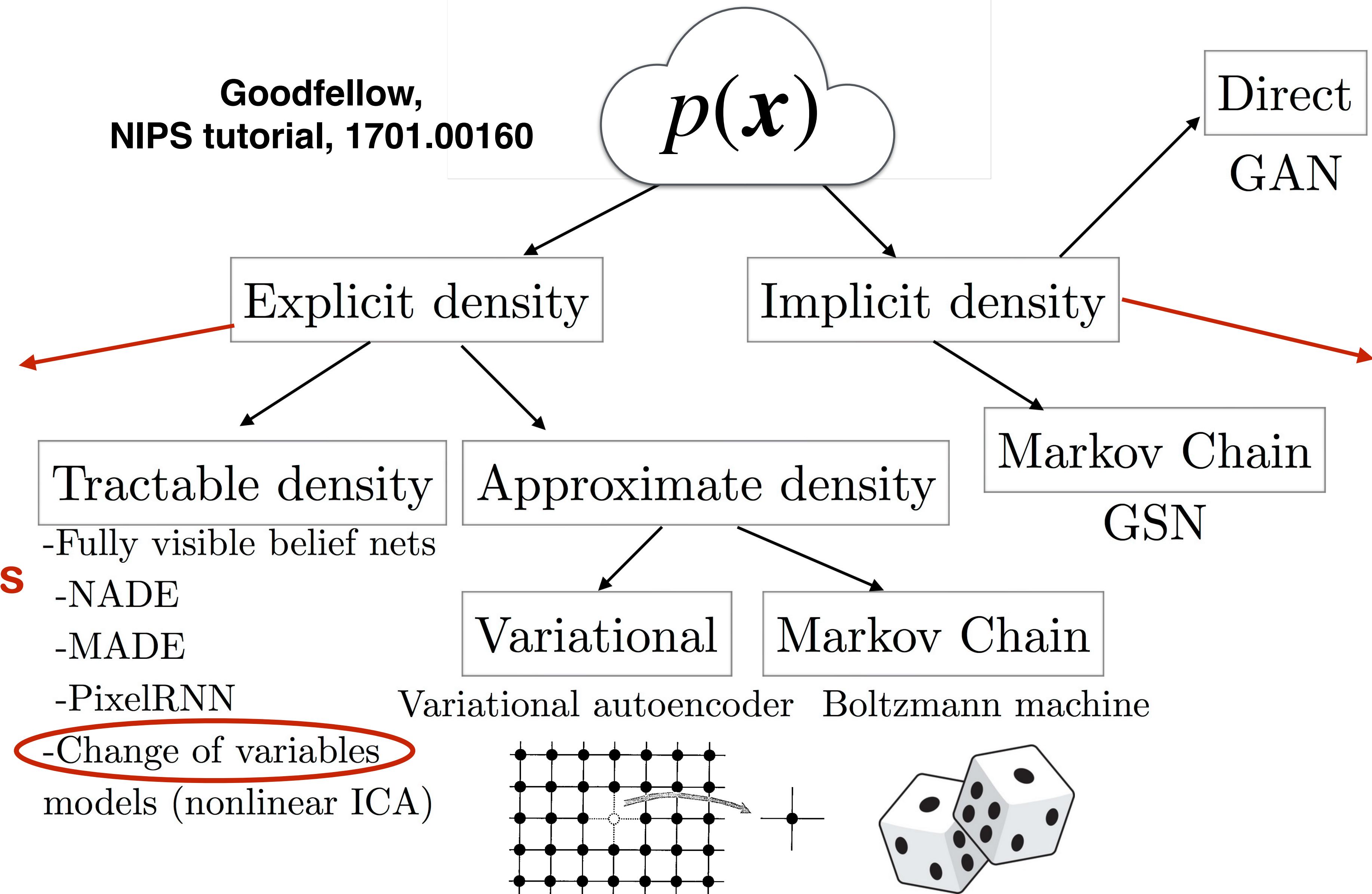
# Physics genes of generative models



Tensor  
Networks



Goodfellow,  
NIPS tutorial, 1701.00160



## Generative Models for Physicists

Lei Wang\*

Institute of Physics, Chinese Academy of Sciences  
Beijing 100190, China

October 28, 2018

### Abstract

Generative models generate unseen samples according to a learned joint probability distribution in the high-dimensional space. They find wide applications in density estimation, variational inference, representation learning and more. Deep generative models and associated techniques (such as differentiable programming and representation learning) are cutting-edge technologies physicists can learn from deep learning.

This note introduces the concept and principles of generative modeling, together with applications of modern generative models (autoregressive models, normalizing flows, variational autoencoders etc) as well as the old ones (Boltzmann machines) to physics problems. As a bonus, this note puts some emphasize on physics-inspired generative models which take insights from statistical, quantum, and fluid mechanics.

The latest version of the note is at <http://wangleiphy.github.io/>. Please send comments, suggestions and corrections to the email address in below.

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# Generative modeling with normalizing flows



Wavenet 1609.03499 1711.10433

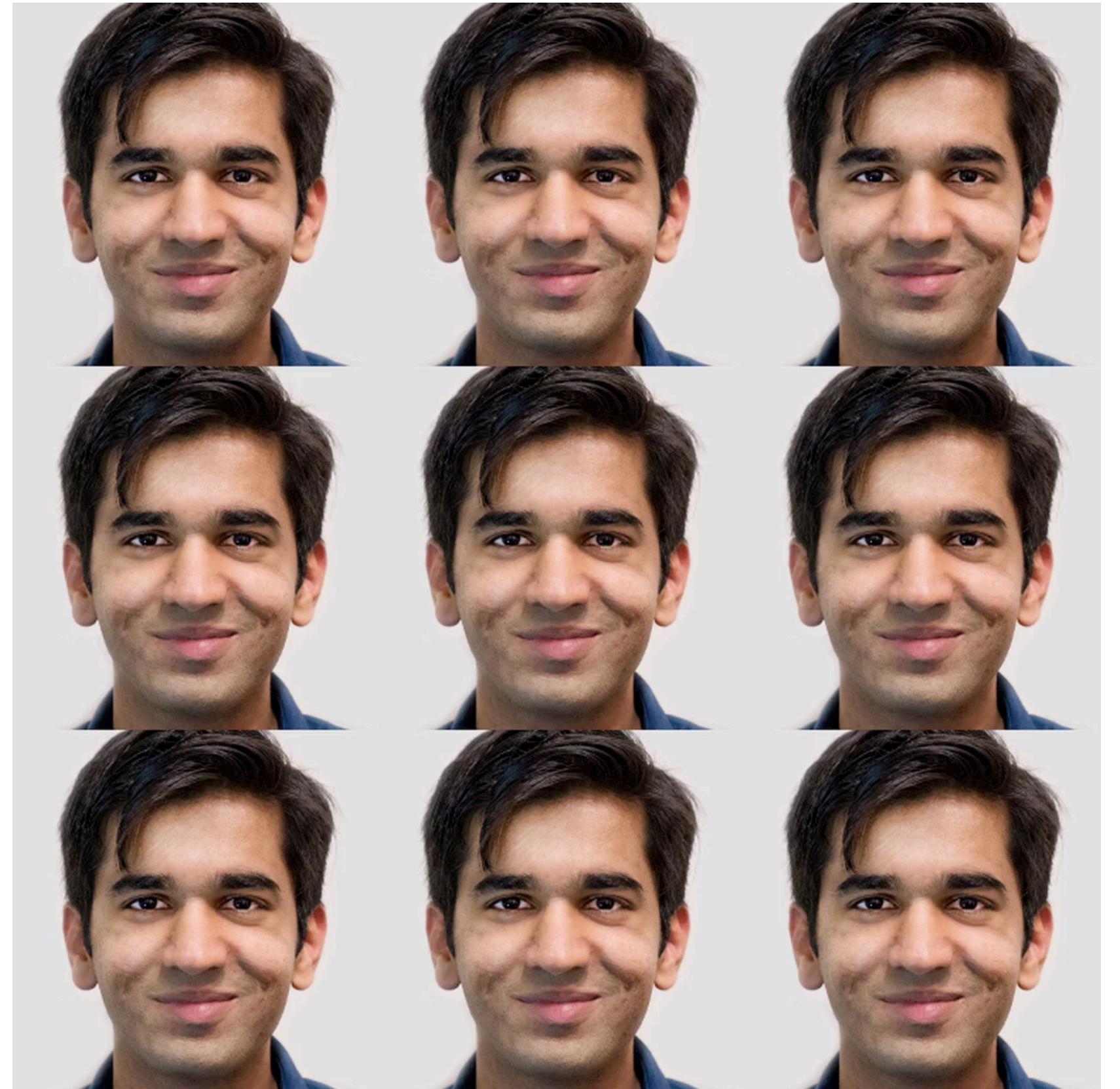
<https://deepmind.com/blog/wavenet-generative-model-raw-audio/>  
<https://deepmind.com/blog/high-fidelity-speech-synthesis-wavenet/>



Glow 1807.03039

<https://blog.openai.com/glow/>

# Generative modeling with normalizing flows



Wavenet 1609.03499 1711.10433

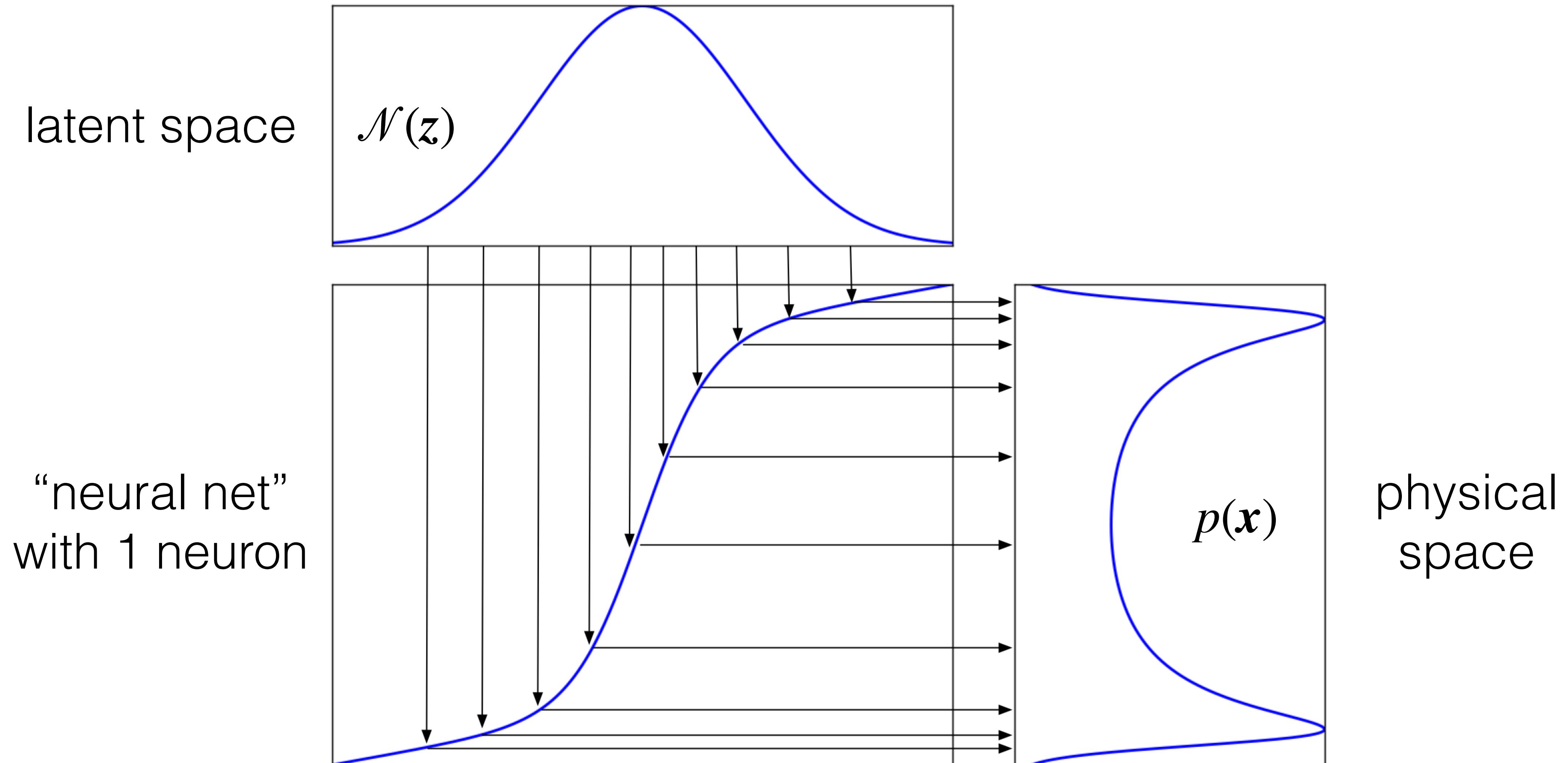
<https://deepmind.com/blog/wavenet-generative-model-raw-audio/>  
<https://deepmind.com/blog/high-fidelity-speech-synthesis-wavenet/>



Glow 1807.03039

<https://blog.openai.com/glow/>

# Normalizing flow in a nutshell



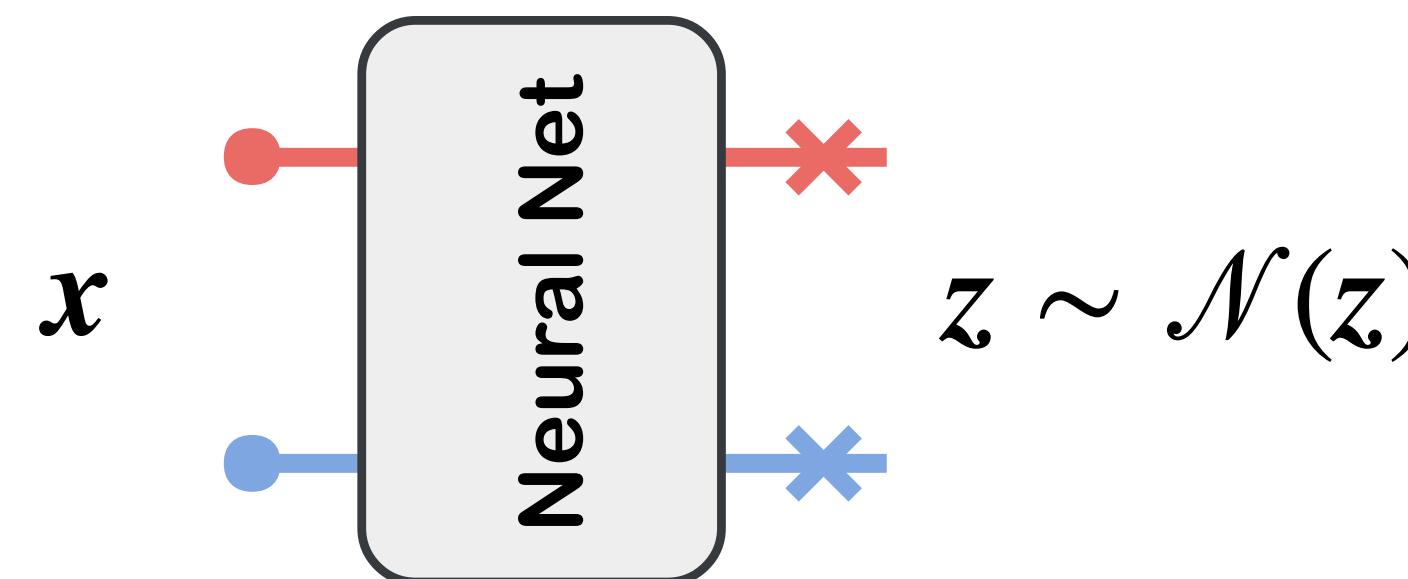
# Normalizing Flows

**Change of variables**  $x \leftrightarrow z$  **with deep neural nets**

$$p(x) = \mathcal{N}(z) \left| \det \left( \frac{\partial z}{\partial x} \right) \right|$$

**Review article** 1912.02762  
**Tutorial** [https://iclr.cc/virtual\\_2020/speaker\\_4.html](https://iclr.cc/virtual_2020/speaker_4.html)

composable, differentiable, and invertible mapping between manifolds



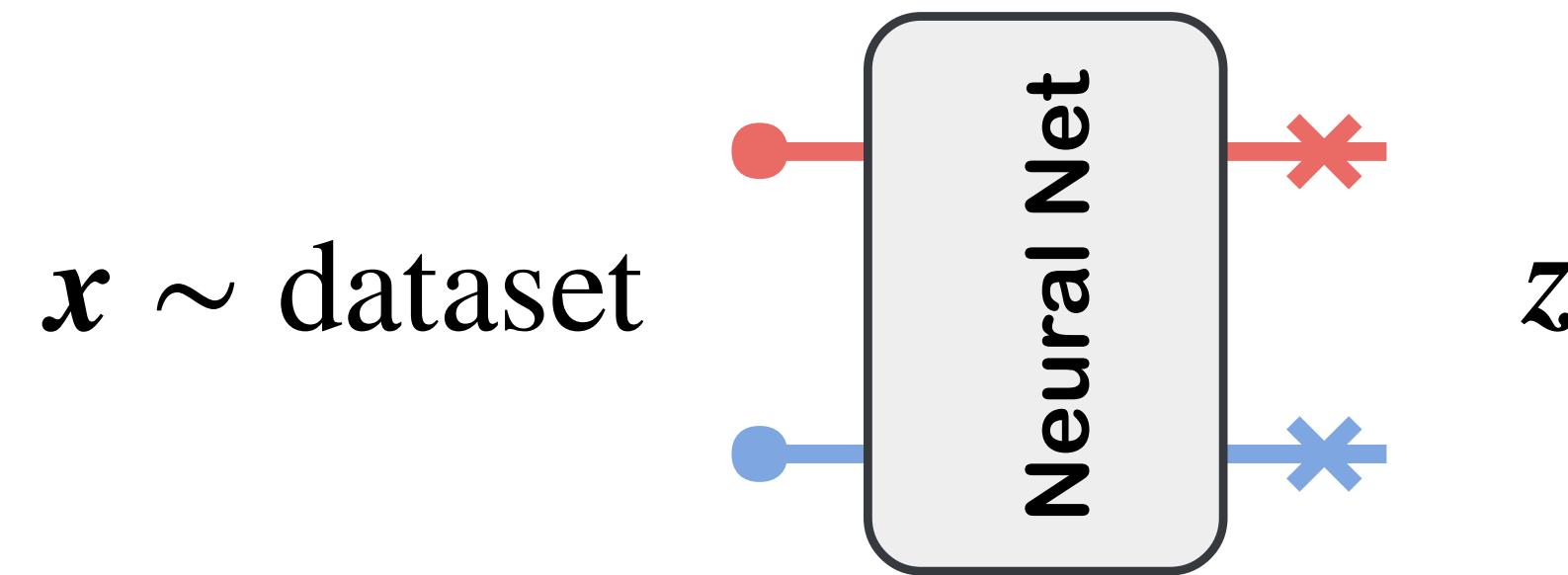
**Learn probability transformations with normalizing flows**

# Training approaches

## Density estimation

“learn from data”

$$\mathcal{L} = - \mathbb{E}_{x \sim \text{dataset}} [\ln p(x)]$$

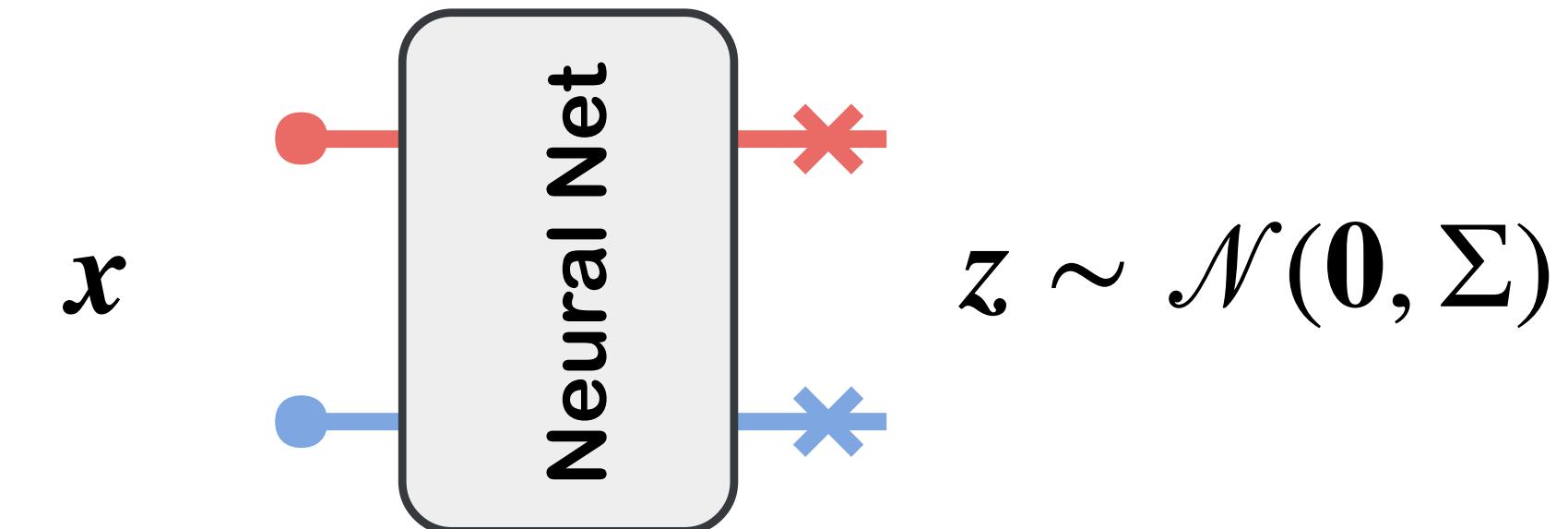


Sample from dataset in the physical space

## Variational calculation

“learn from Hamiltonian”

$$\mathcal{L} = \int dx p(x) [\ln p(x) + \beta H(x)]$$



Sample in the latent space

# Training approaches

## Density estimation

“learn from data”

$$\mathcal{L} = -\mathbb{E}_{x \sim \text{dataset}} [\ln p(x)]$$

$$\mathbb{KL}(\pi || p) = \sum_x \underbrace{\pi \ln \pi - \sum_x \pi \ln p}_{\mathcal{L}}$$

Sample from dataset in the physical space

## Variational calculation

“learn from Hamiltonian”

$$\mathcal{L} = \int dx p(x) [\ln p(x) + \beta H(x)]$$

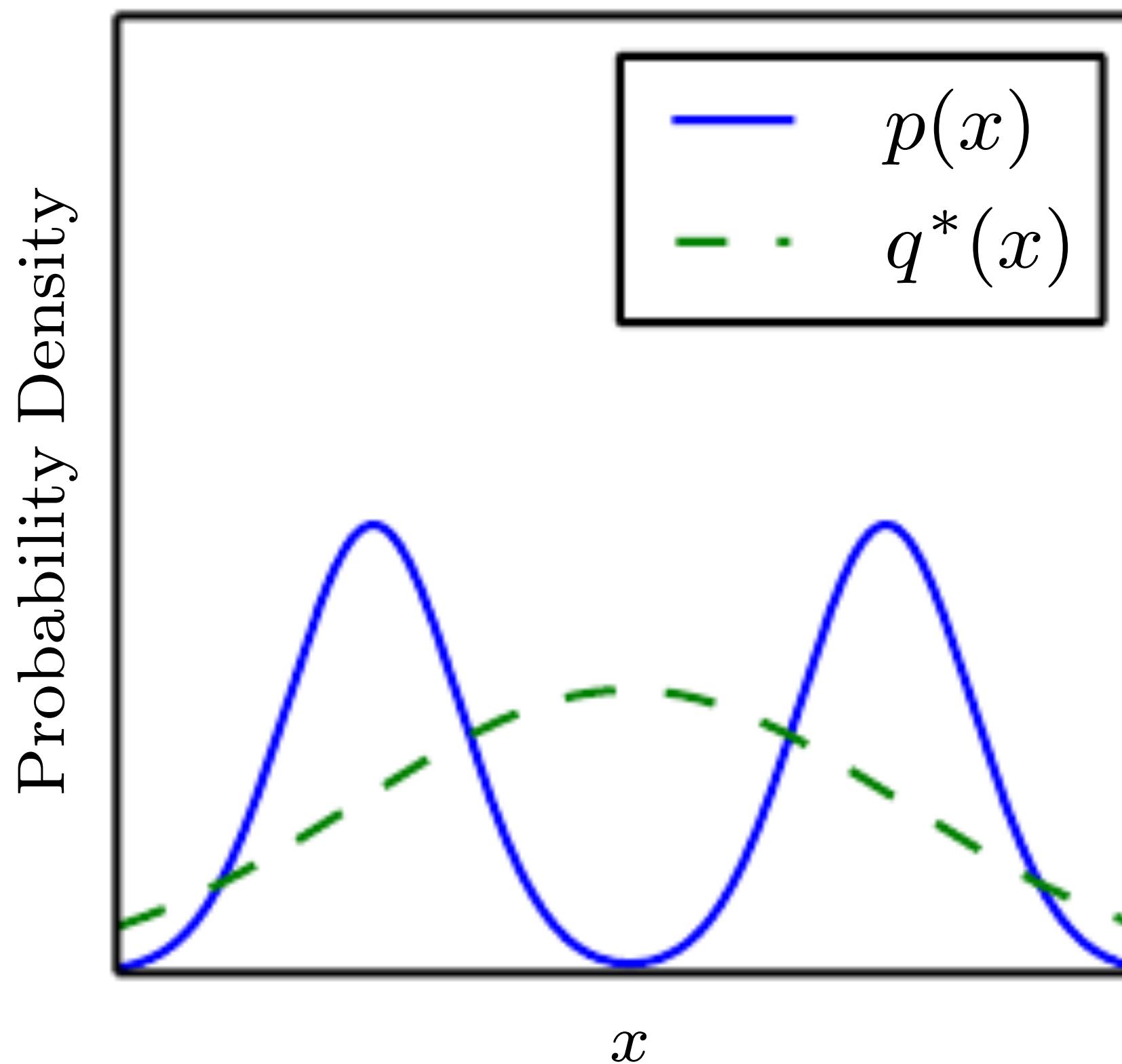
$$\mathcal{L} + \ln Z = \mathbb{KL} \left( p || \frac{e^{-\beta H}}{Z} \right) \geq 0$$

Sample in the latent space

# Forward KL or Reverse KL ?

## Maximum Likelihood Estimation

$$q^* = \operatorname{argmin}_q D_{\text{KL}}(p\|q)$$



## Variational Free Energy

$$q^* = \operatorname{argmin}_q D_{\text{KL}}(q\|p)$$

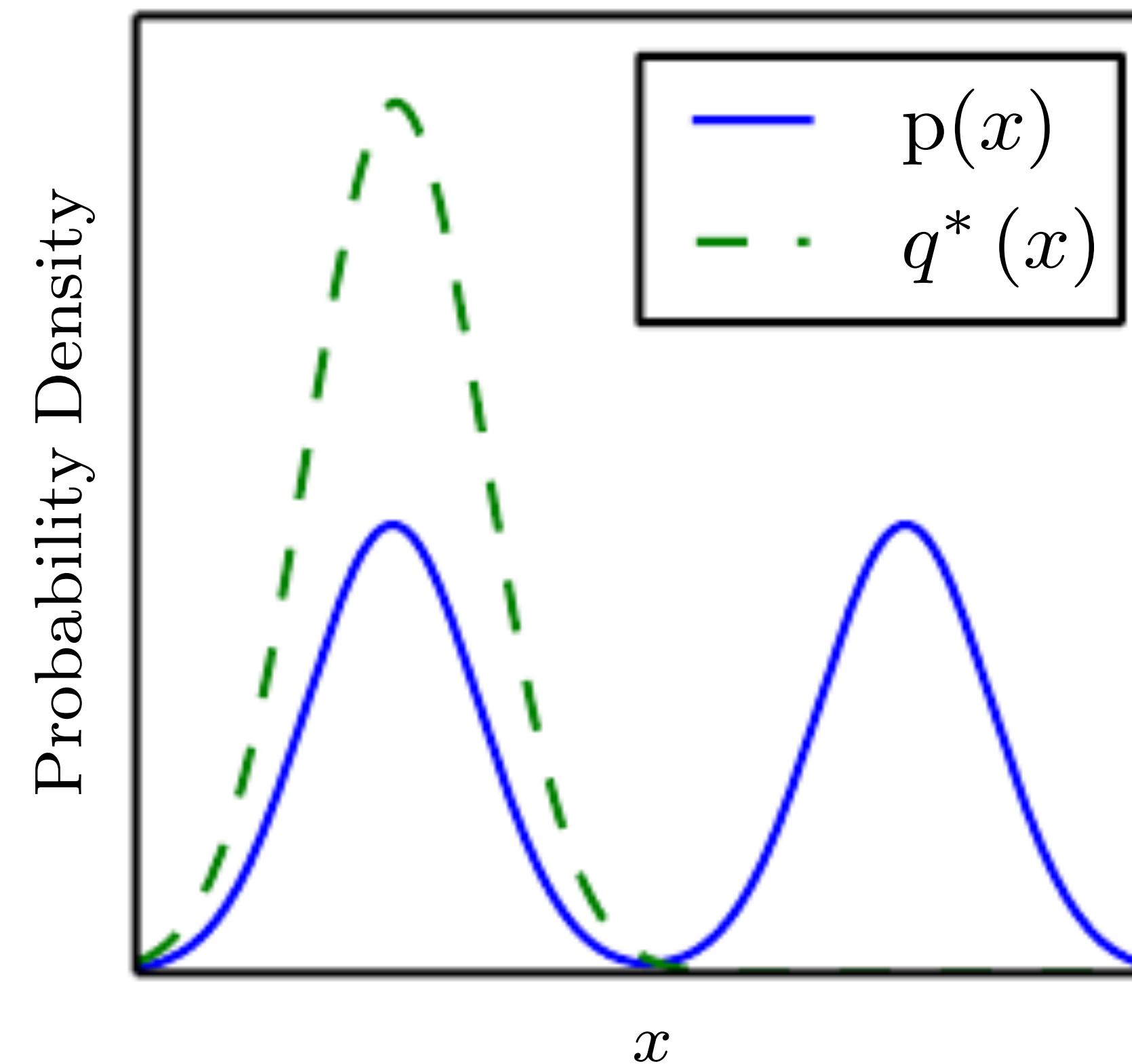


Fig. 3.6, Goodfellow, Bengio, Courville, <http://www.deeplearningbook.org/>

# Monte Carlo Gradient Estimators

**Review: 1906.10652**

$$\nabla_{\theta} \mathbb{E}_{x \sim p_{\theta}} [f(x)]$$

Reinforcement learning

Variational inference

Variational Monte Carlo

Variational quantum algorithms

...

Score function estimator (REINFORCE)

$$\nabla_{\theta} \mathbb{E}_{x \sim p_{\theta}} [f(x)] = \mathbb{E}_{x \sim p_{\theta}} [f(x) \nabla_{\theta} \ln p_{\theta}(x)]$$

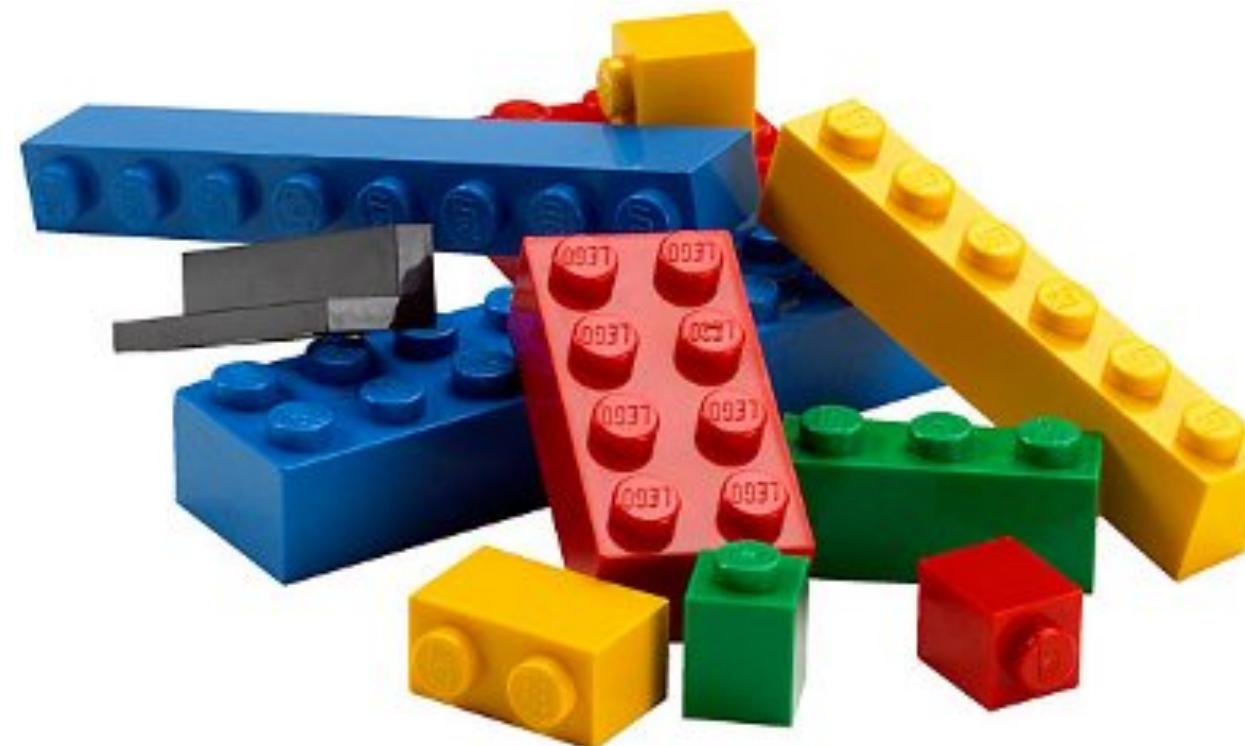
Pathwise estimator (Reparametrization trick)  $x = g_{\theta}(z)$

$$\nabla_{\theta} \mathbb{E}_{x \sim p_{\theta}} [f(x)] = \mathbb{E}_{z \sim \mathcal{N}(z)} [\nabla_{\theta} f(g_{\theta}(z))]$$

**Choose the one with the lowest variance**

# Design principles

**Composability**

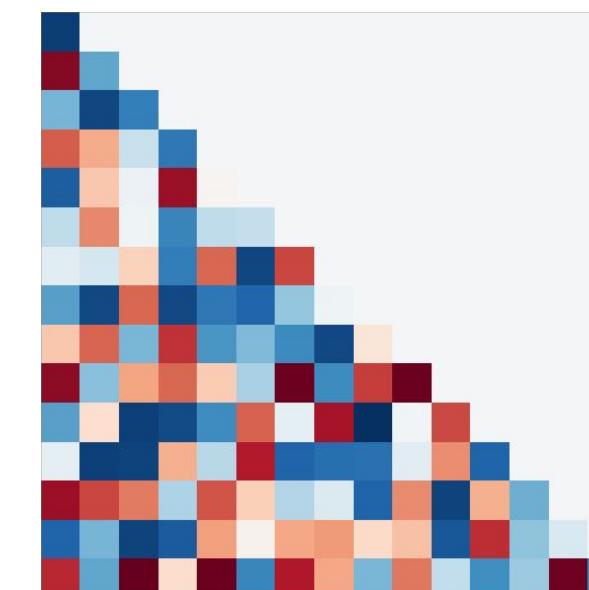


$$z = \mathcal{T}(x)$$

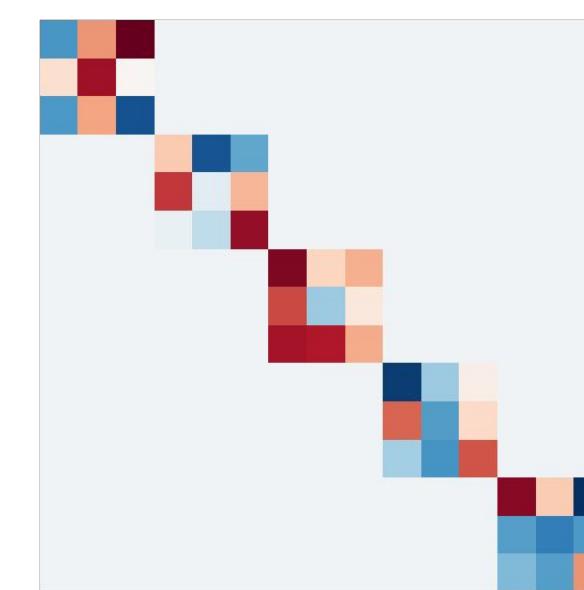
$$\mathcal{T} = \mathcal{T}_1 \circ \mathcal{T}_2 \circ \mathcal{T}_3 \circ \dots$$

**Balanced  
efficiency &  
inductive bias**

$$\left| \det \left( \frac{\partial z}{\partial x} \right) \right|$$



Autoregressive



Neural RG

$$\frac{\partial \rho(x, t)}{\partial t} + \nabla \cdot [\rho(x, t)v] = 0$$

Continuous flow

# Example of a building block

Forward

$$\begin{cases} \mathbf{x}_< = \mathbf{z}_< \\ \mathbf{x}_> = \mathbf{z}_> \odot e^{s(\mathbf{z}_<)} + t(\mathbf{z}_<) \end{cases}$$

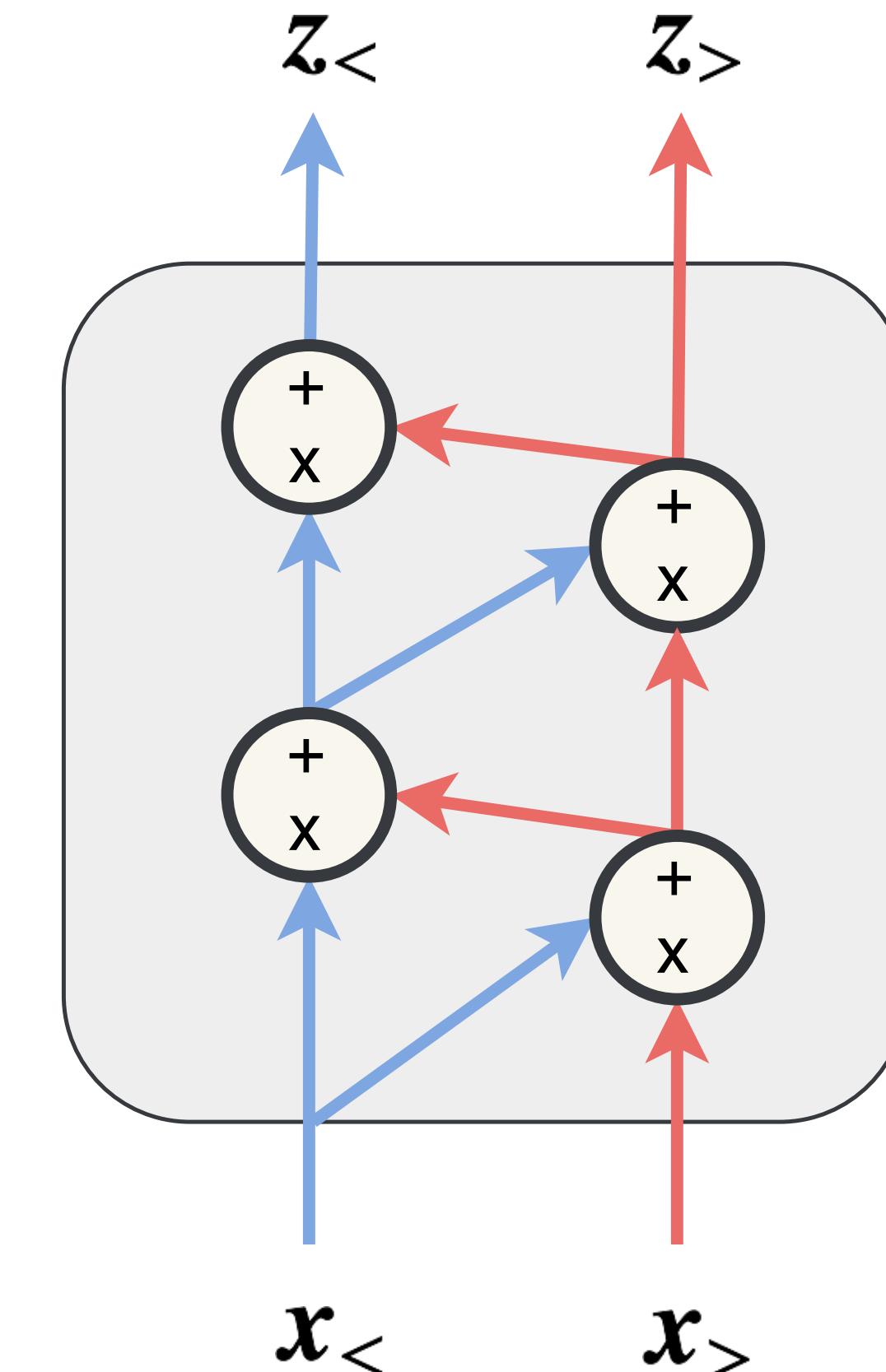
arbitrary  
neural nets

Inverse

$$\begin{cases} \mathbf{z}_< = \mathbf{x}_< \\ \mathbf{z}_> = (\mathbf{x}_> - t(\mathbf{x}_<)) \odot e^{-s(\mathbf{x}_<)} \end{cases}$$

Log-Abs-Jacobian-Det

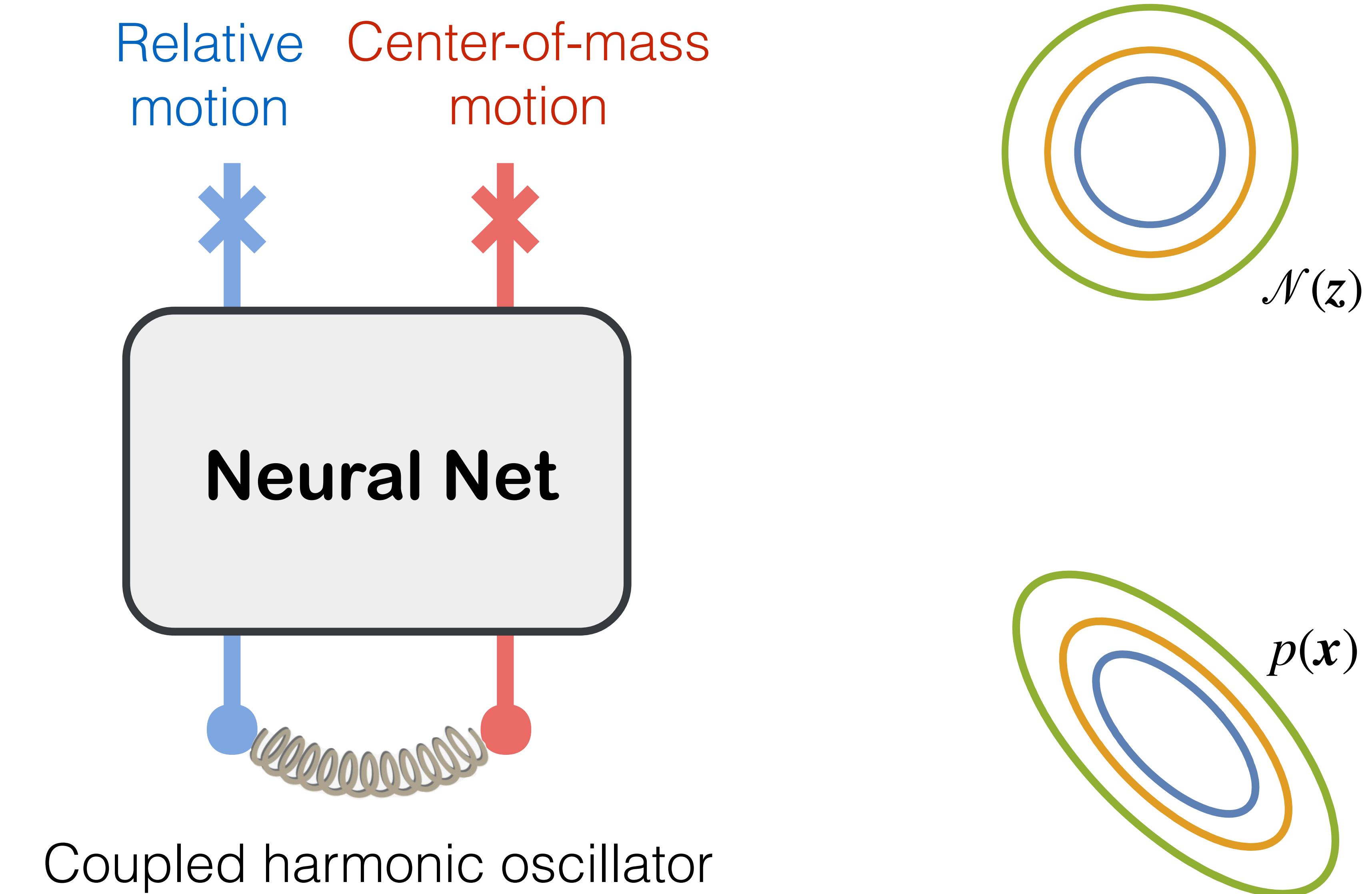
$$\ln \left| \det \left( \frac{\partial \mathbf{x}}{\partial \mathbf{z}} \right) \right| = \sum_i [s(\mathbf{z}_<)]_i$$



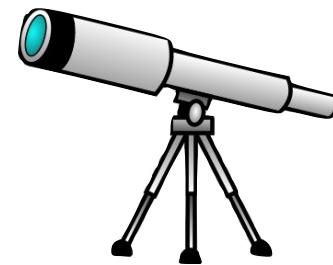
Real NVP, Dinh et al, 1605.08803

Turns out to have surprising connection Störmer–Verlet integration (later)

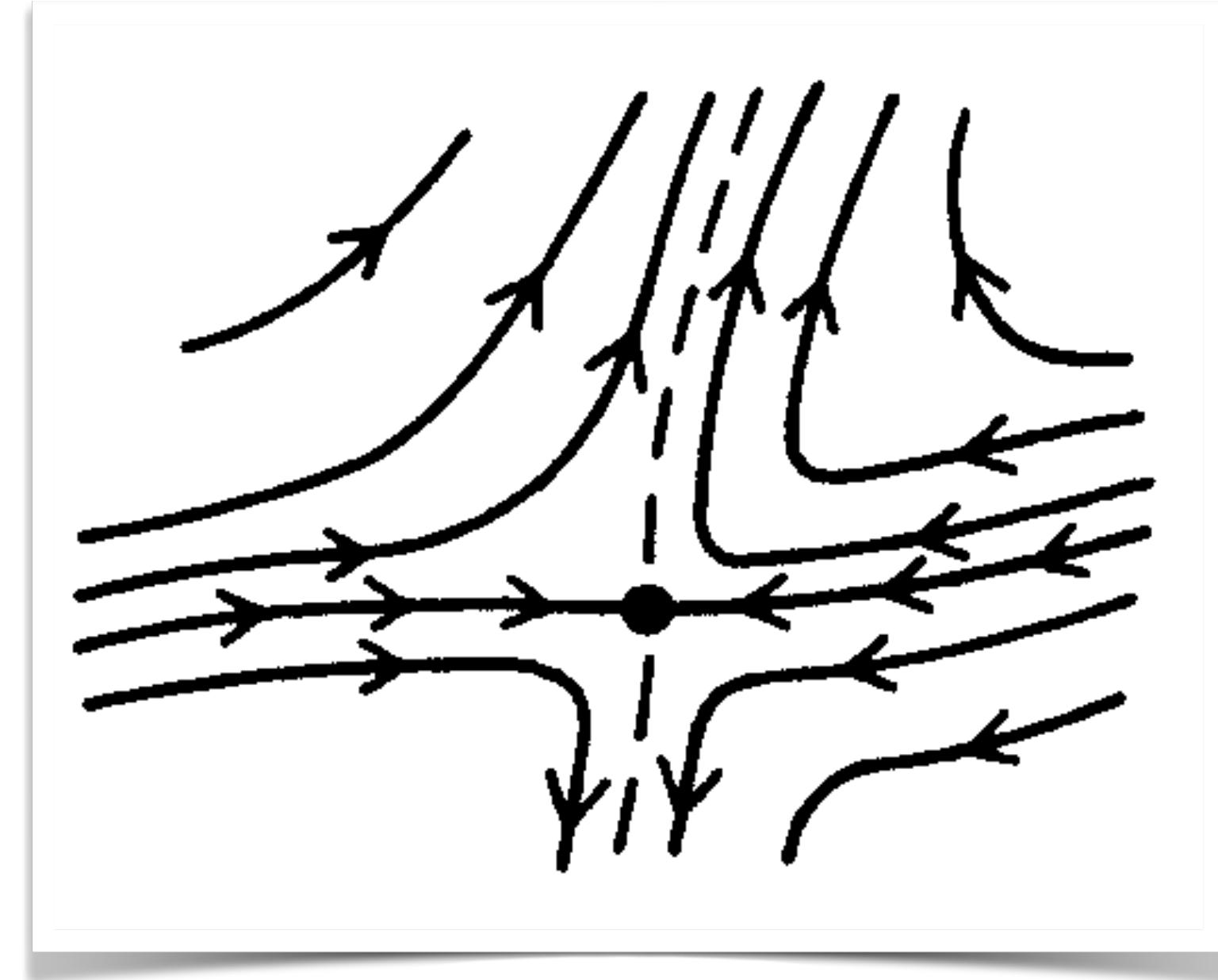
# How it can be useful in physics ?



# How it can be useful in physics ?



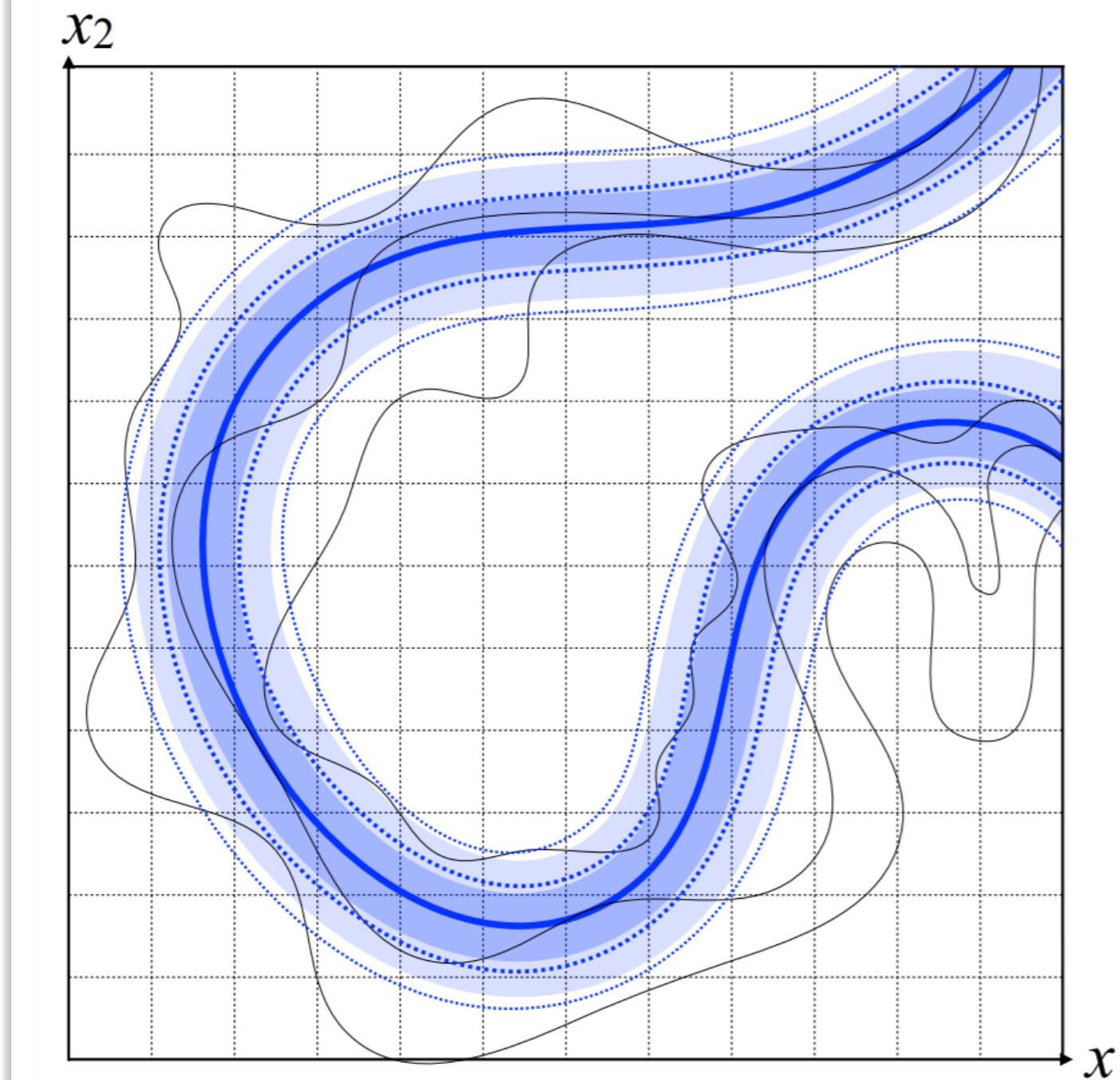
## Renormalization group



Effective theory emerges upon transformation of the variables



## Monte Carlo update

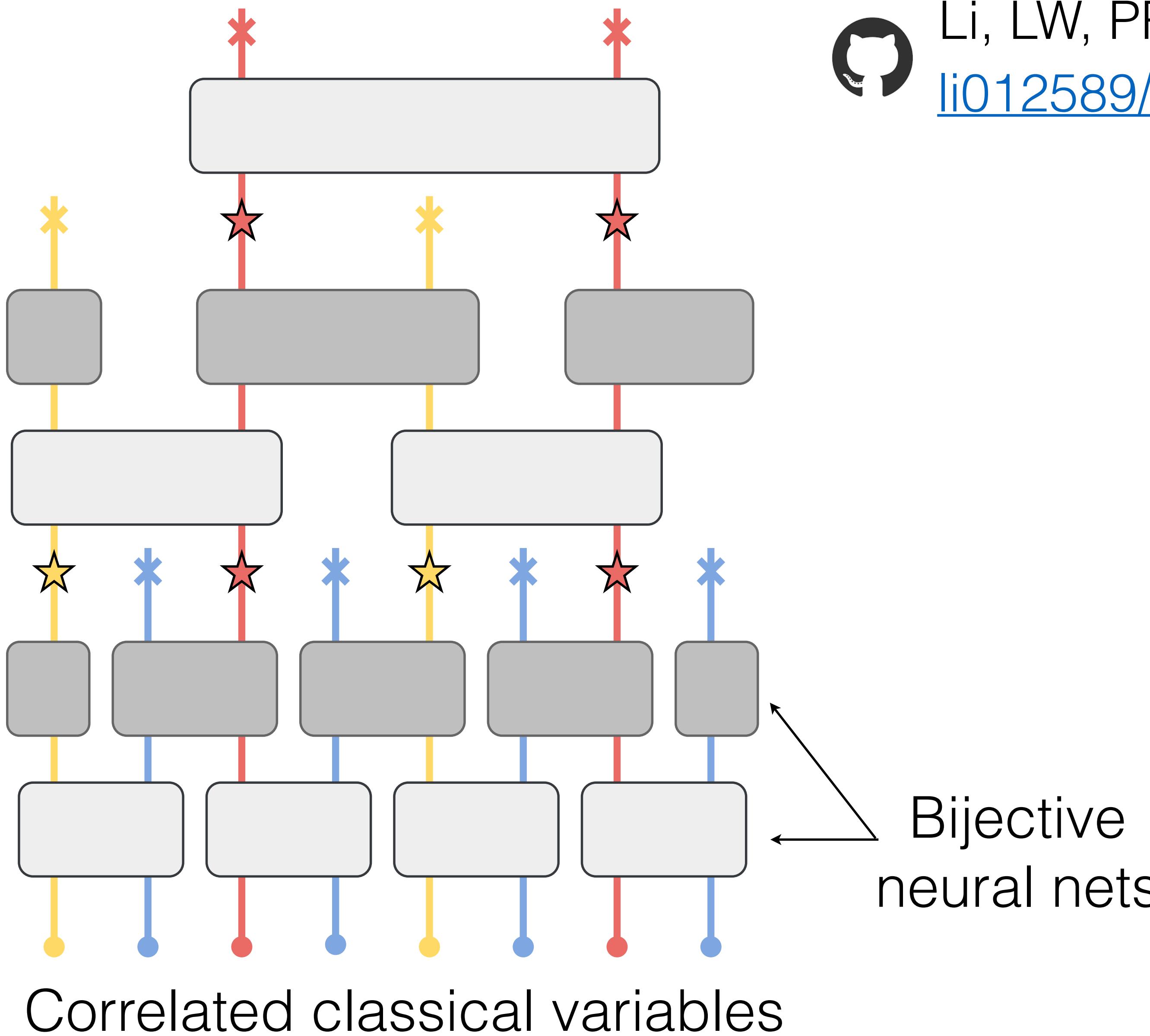


Physics happens on a manifold  
Learn neural nets to unfold that manifold

# Neural Network Renormalization Group



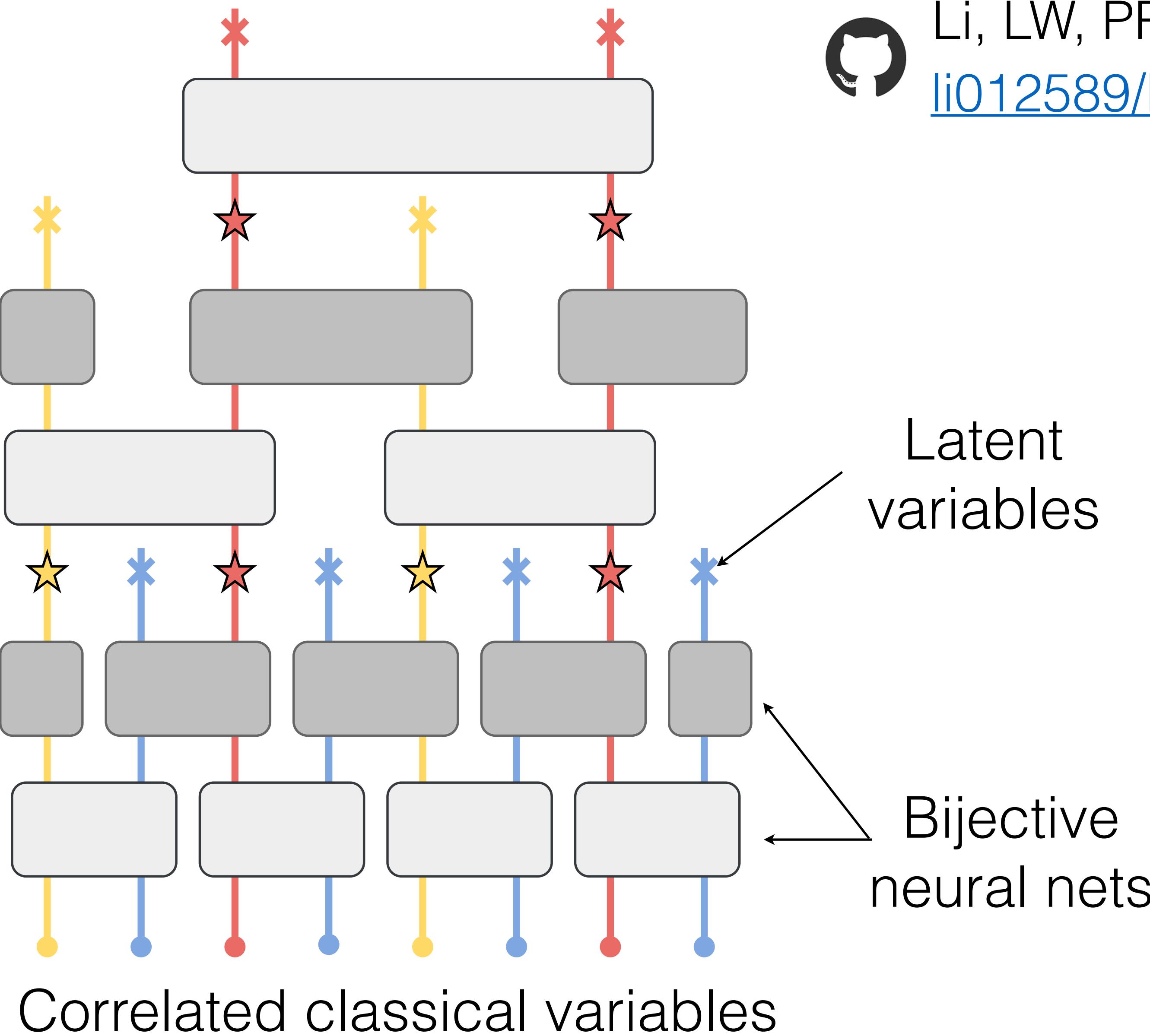
Li, LW, PRL '18  
[li012589/NeuralRG](https://github.com/li012589/NeuralRG)



# Neural Network Renormalization Group



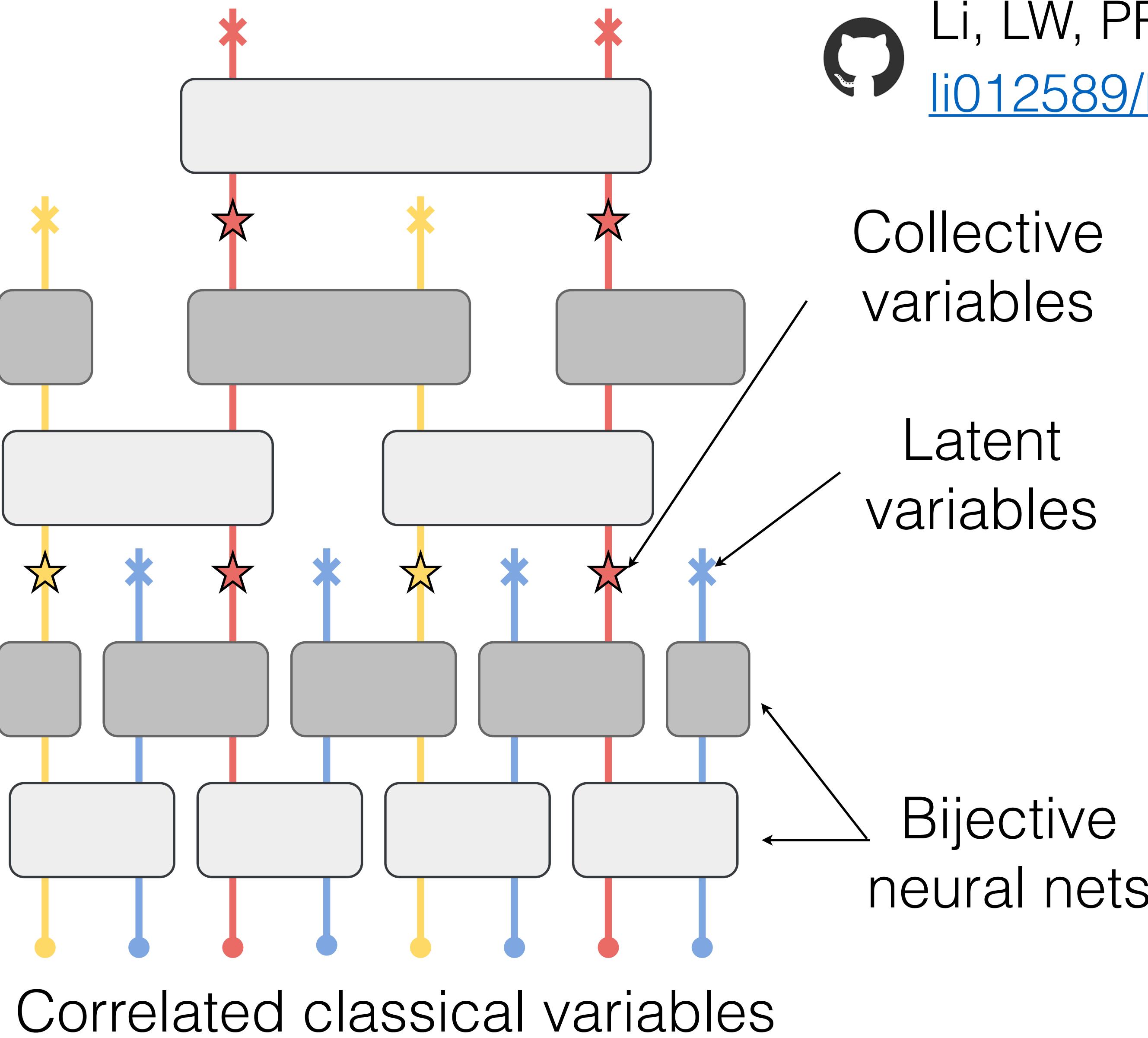
Li, LW, PRL '18  
[li012589/NeuralRG](https://github.com/li012589/NeuralRG)



# Neural Network Renormalization Group

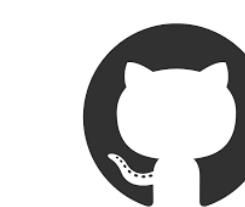
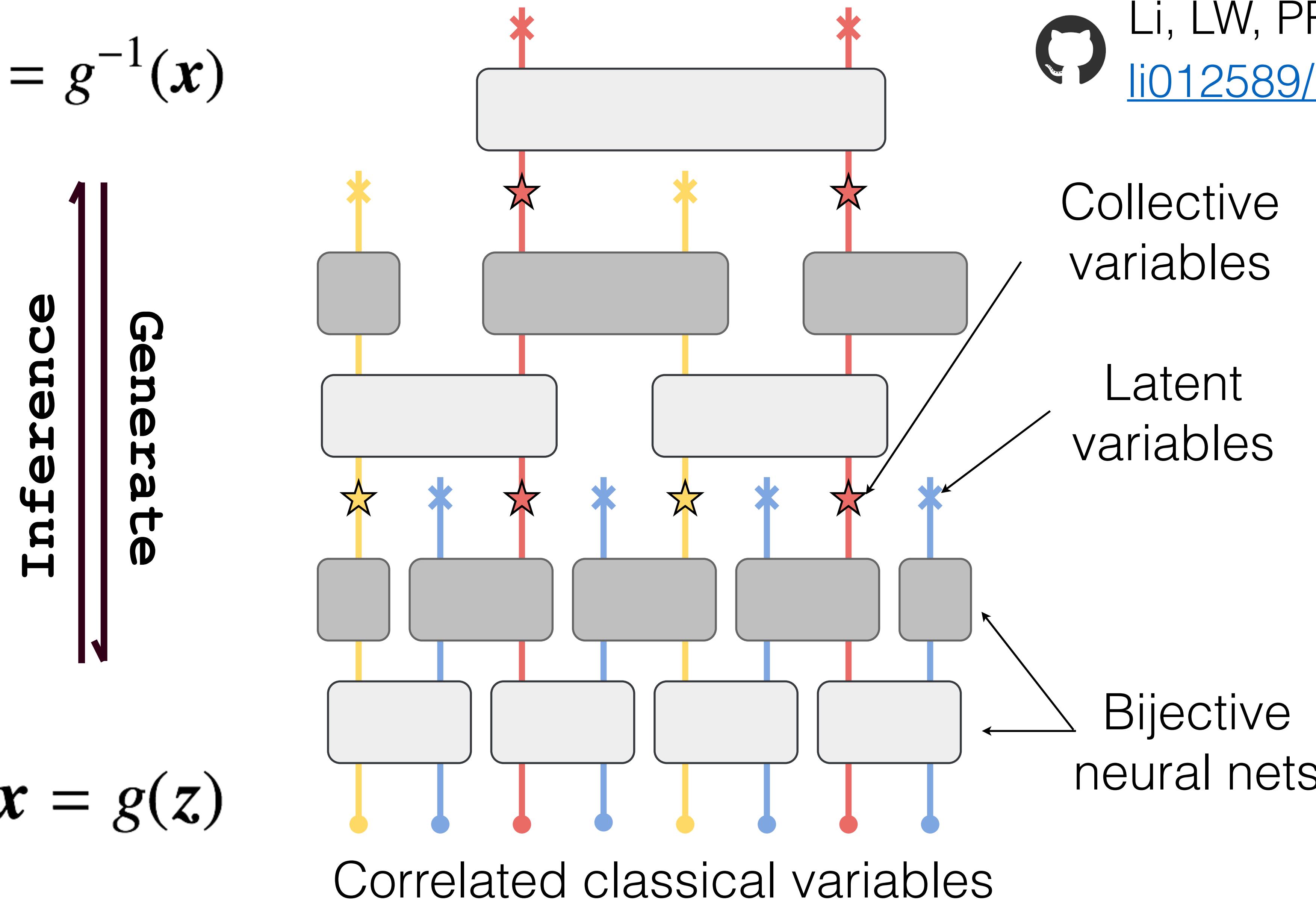


Li, LW, PRL '18  
[li012589/NeuralRG](https://github.com/li012589/NeuralRG)



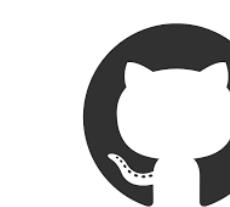
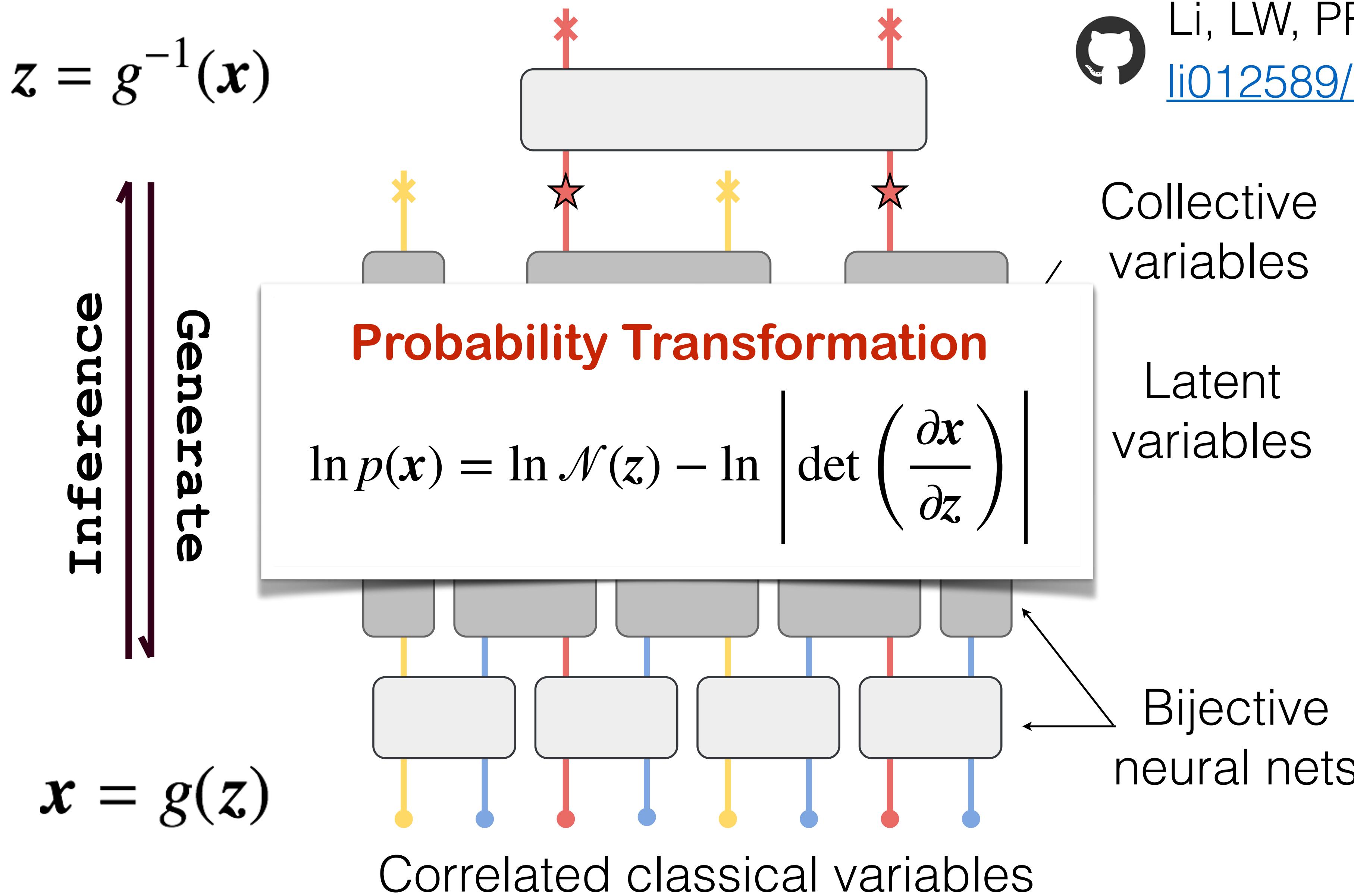
# Neural Network Renormalization Group

$$z = g^{-1}(x)$$



Li, LW, PRL '18  
[li012589/NeuralRG](https://arxiv.org/abs/1803.03984)

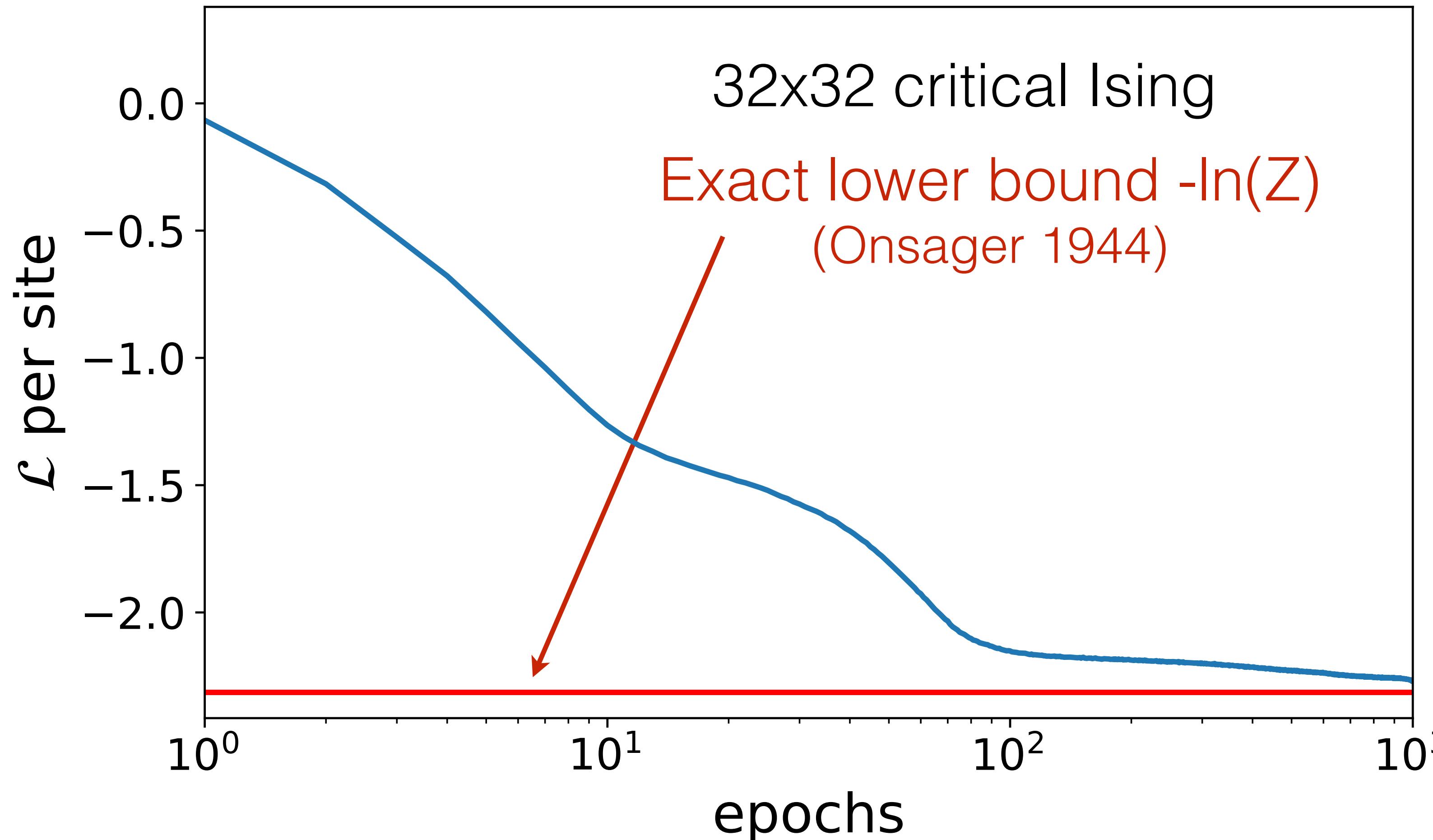
# Neural Network Renormalization Group



Li, LW, PRL '18

[li012589/NeuralRG](https://arxiv.org/abs/1803.03311)

# Variational Loss

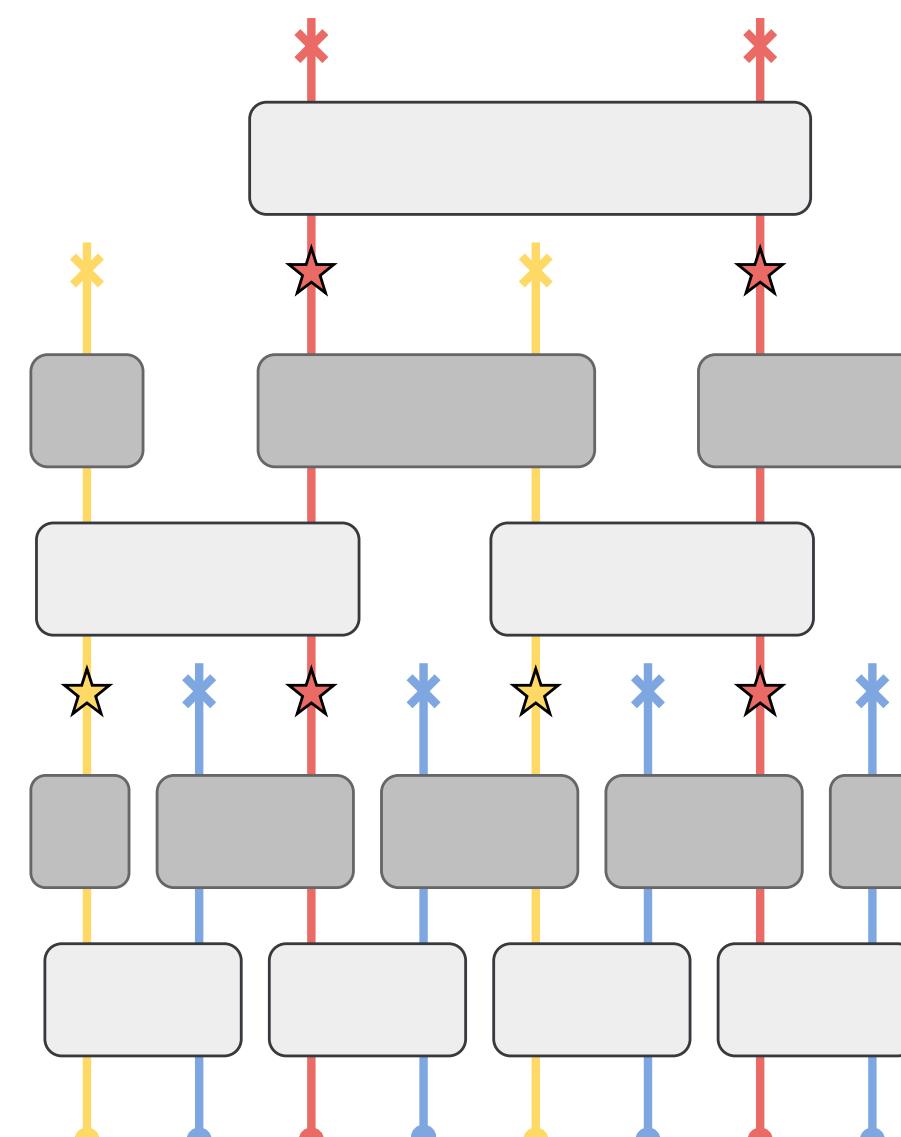


Training = Variational free energy calculation

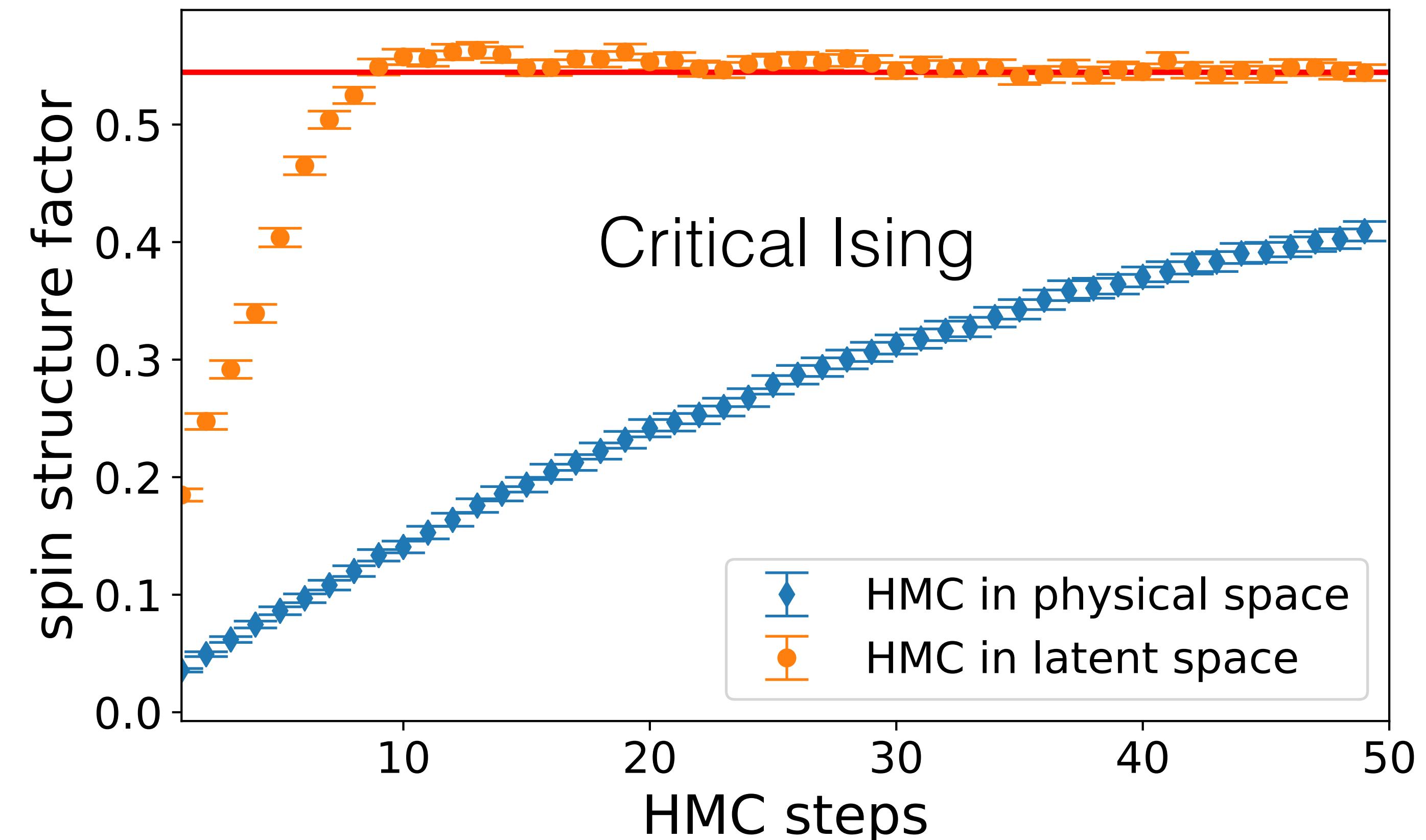
# Sampling in the latent space

Latent space energy function

$$E_{\text{eff}}(z) = E(g(z)) + \ln p(g(z)) - \ln \mathcal{N}(z)$$



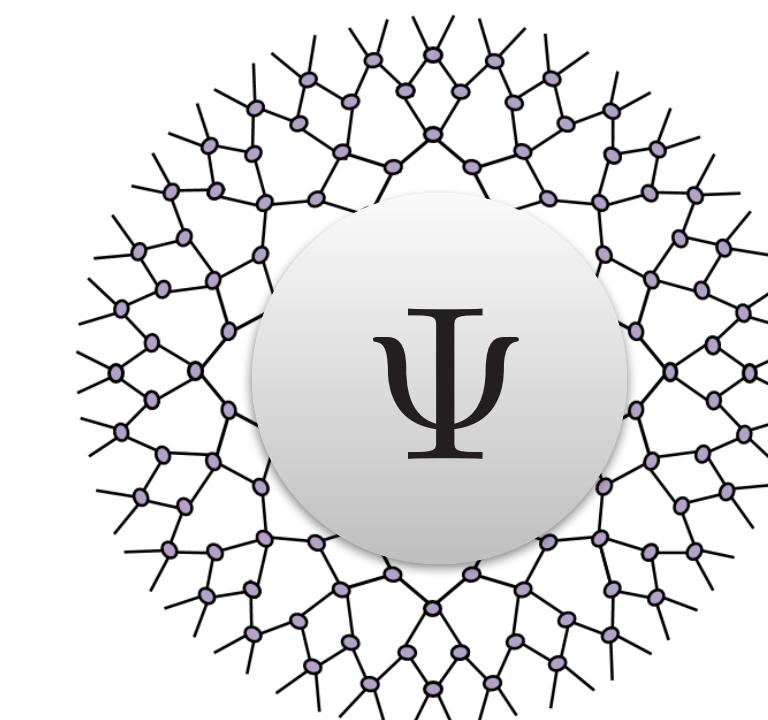
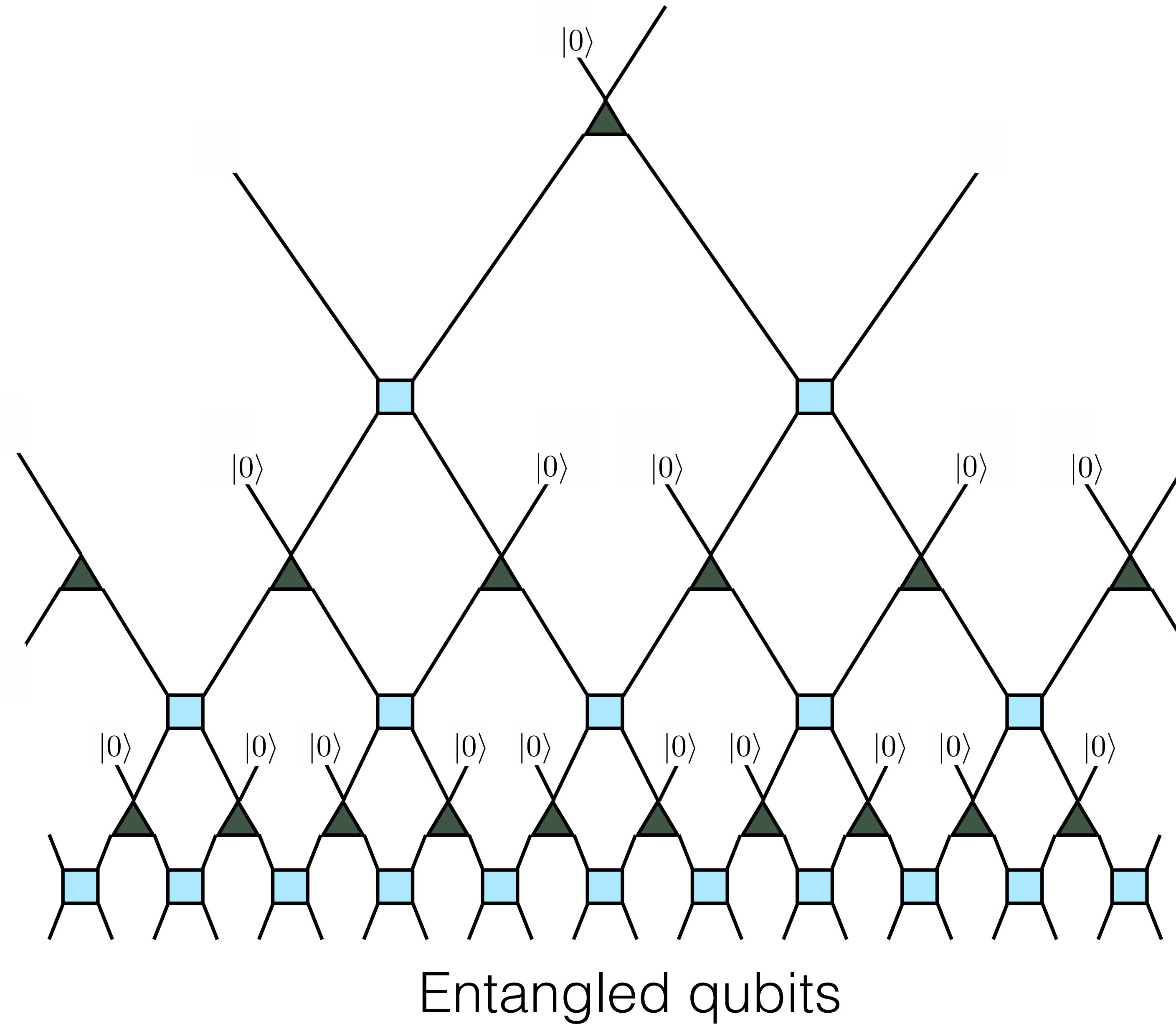
Physical energy function  $E(x)$



**HMC thermalizes faster in the latent space**

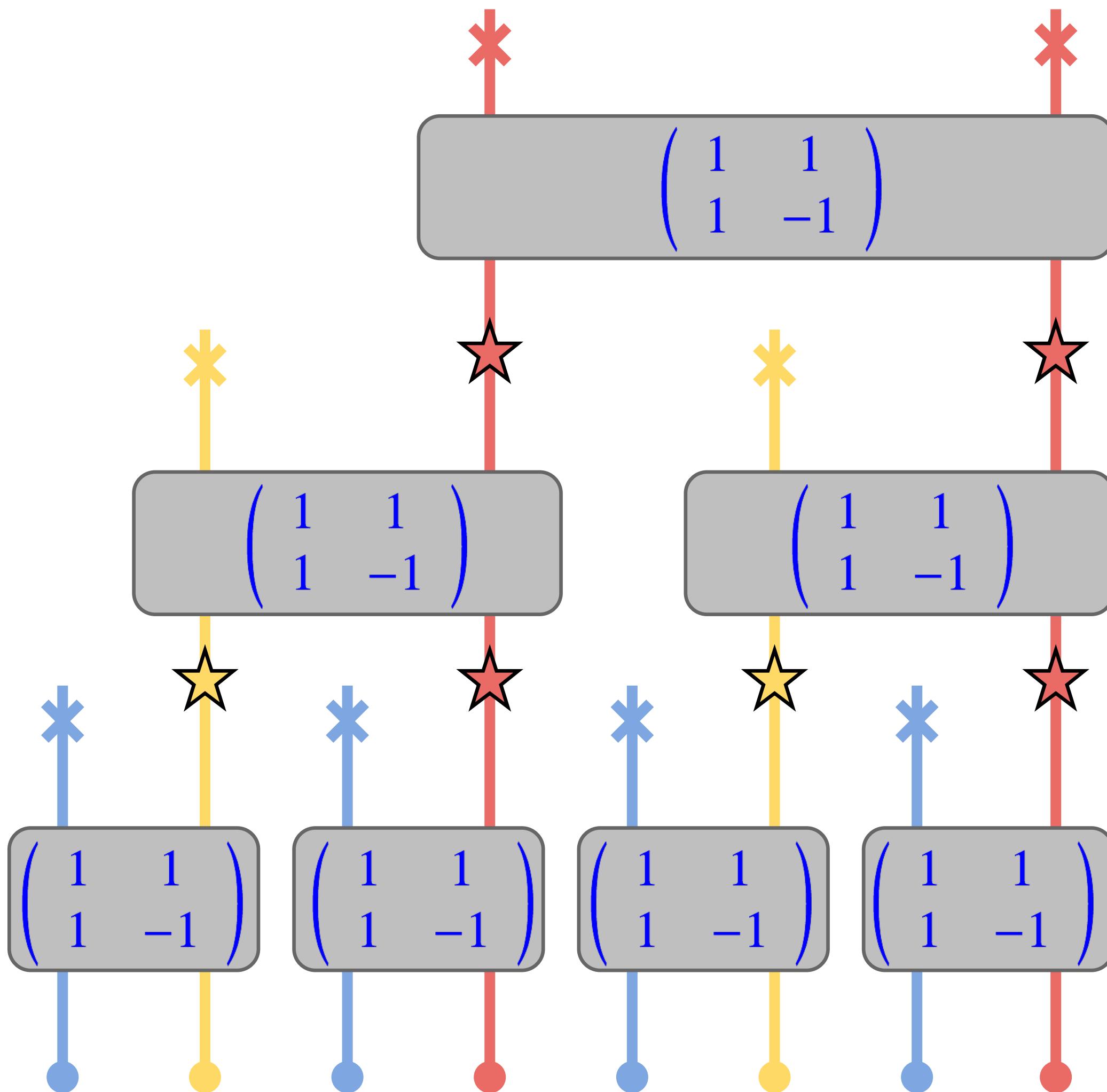
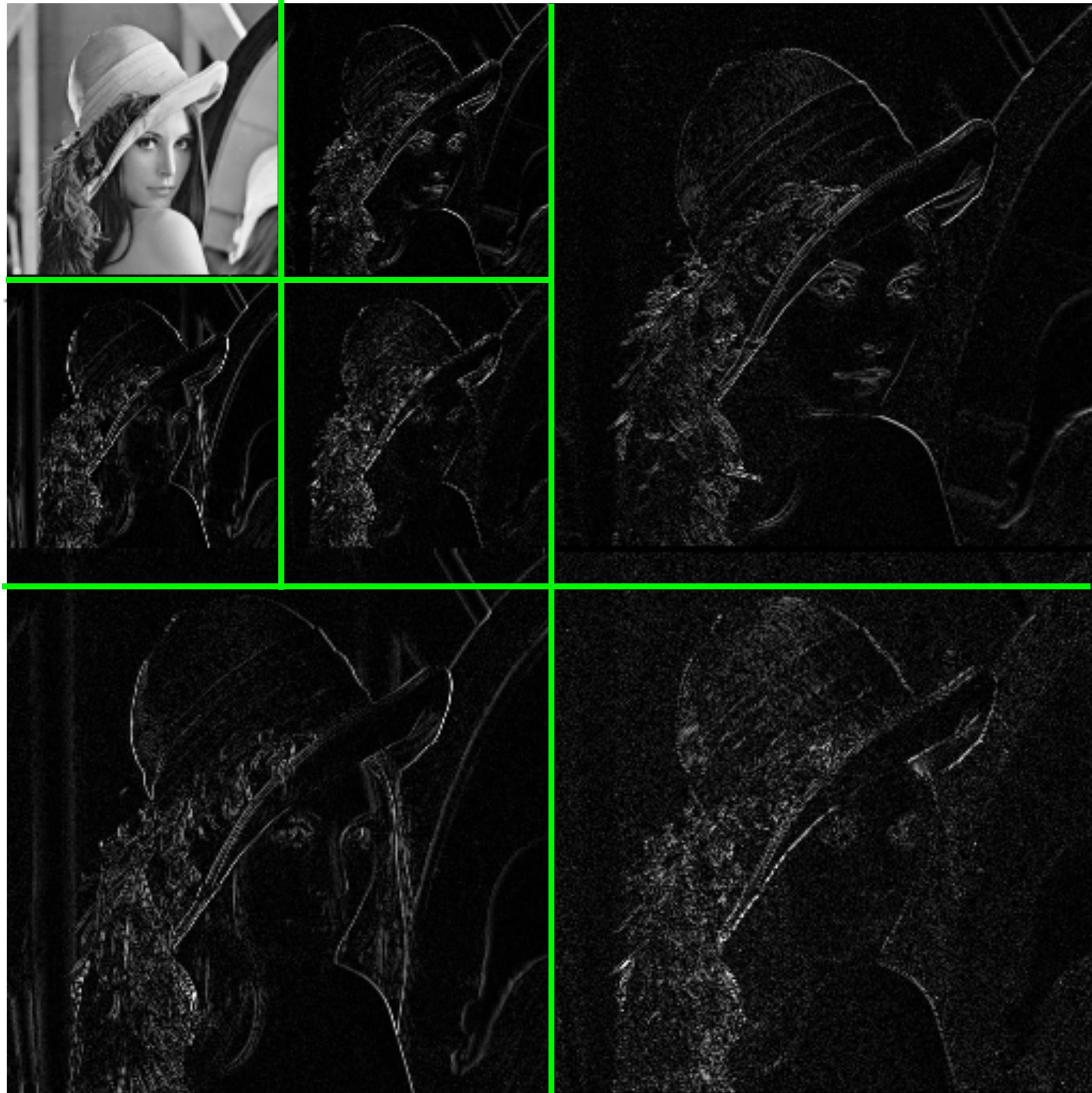
Other ways to de-bias: neural importance sampling, Metropolis rejection of flow proposal ...

# Quantum origin of the architecture



**M**ulti-Scale  
**E**ntanglement  
**R**enormalization  
**A**nsatz

# Connection to wavelets



**Nonlinear & adaptive generalizations of wavelets**

# Continuous normalizing flows

$$\ln p(\mathbf{x}) = \ln \mathcal{N}(\mathbf{z}) - \ln \left| \det \left( \frac{\partial \mathbf{x}}{\partial \mathbf{z}} \right) \right|$$

Consider infinitesimal change-of-variables Chen et al 1806.07366

$$\mathbf{x} = \mathbf{z} + \varepsilon \boldsymbol{\nu}$$

$$\ln p(\mathbf{x}) - \ln \mathcal{N}(\mathbf{z}) = - \ln \left| \det \left( 1 + \varepsilon \frac{\partial \boldsymbol{\nu}}{\partial \mathbf{z}} \right) \right|$$

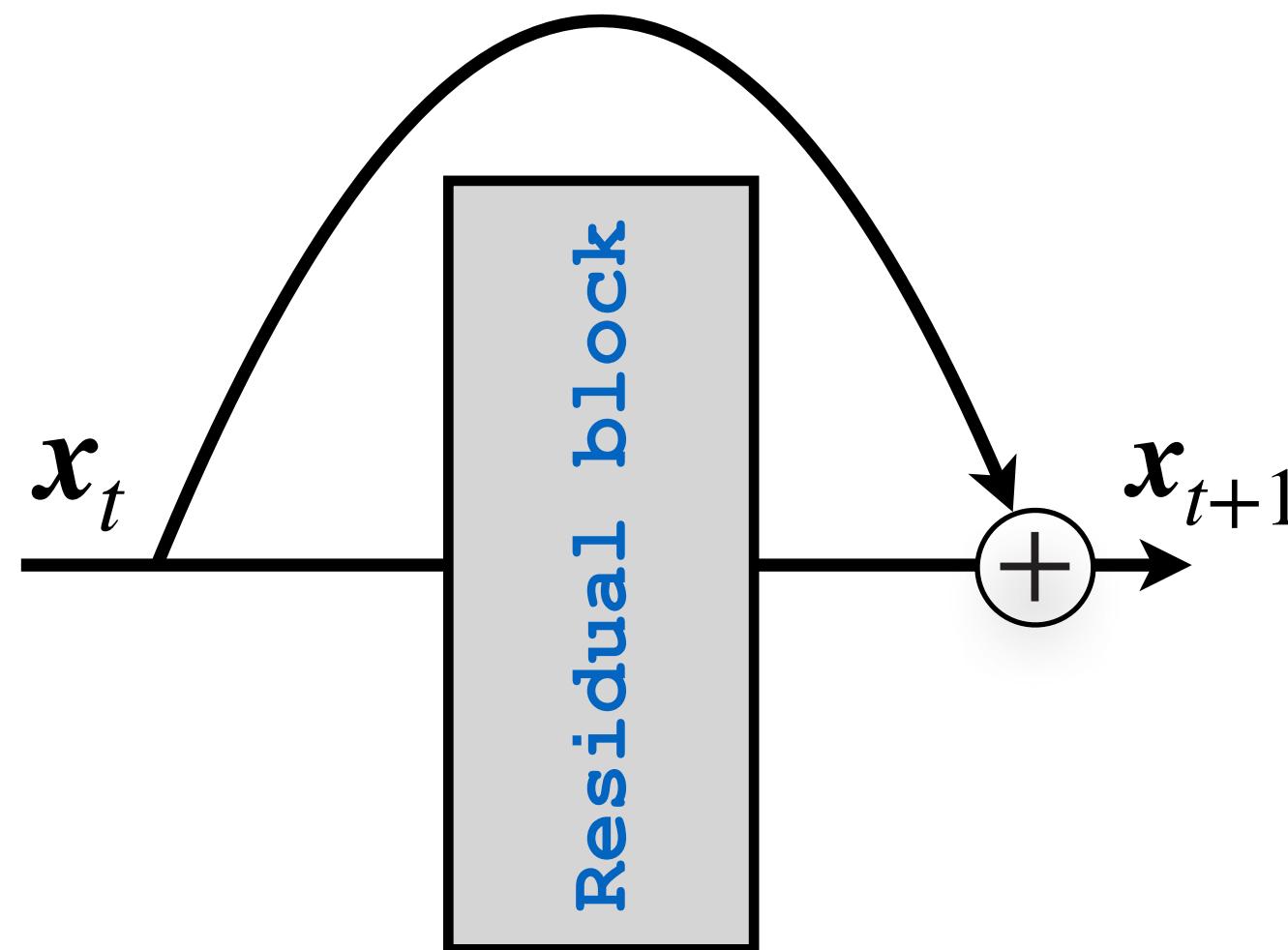
$$\varepsilon \rightarrow 0$$

$$\frac{d\mathbf{x}}{dt} = \boldsymbol{\nu}$$

$$\frac{d \ln \rho(\mathbf{x}, t)}{dt} = - \nabla \cdot \boldsymbol{\nu}$$

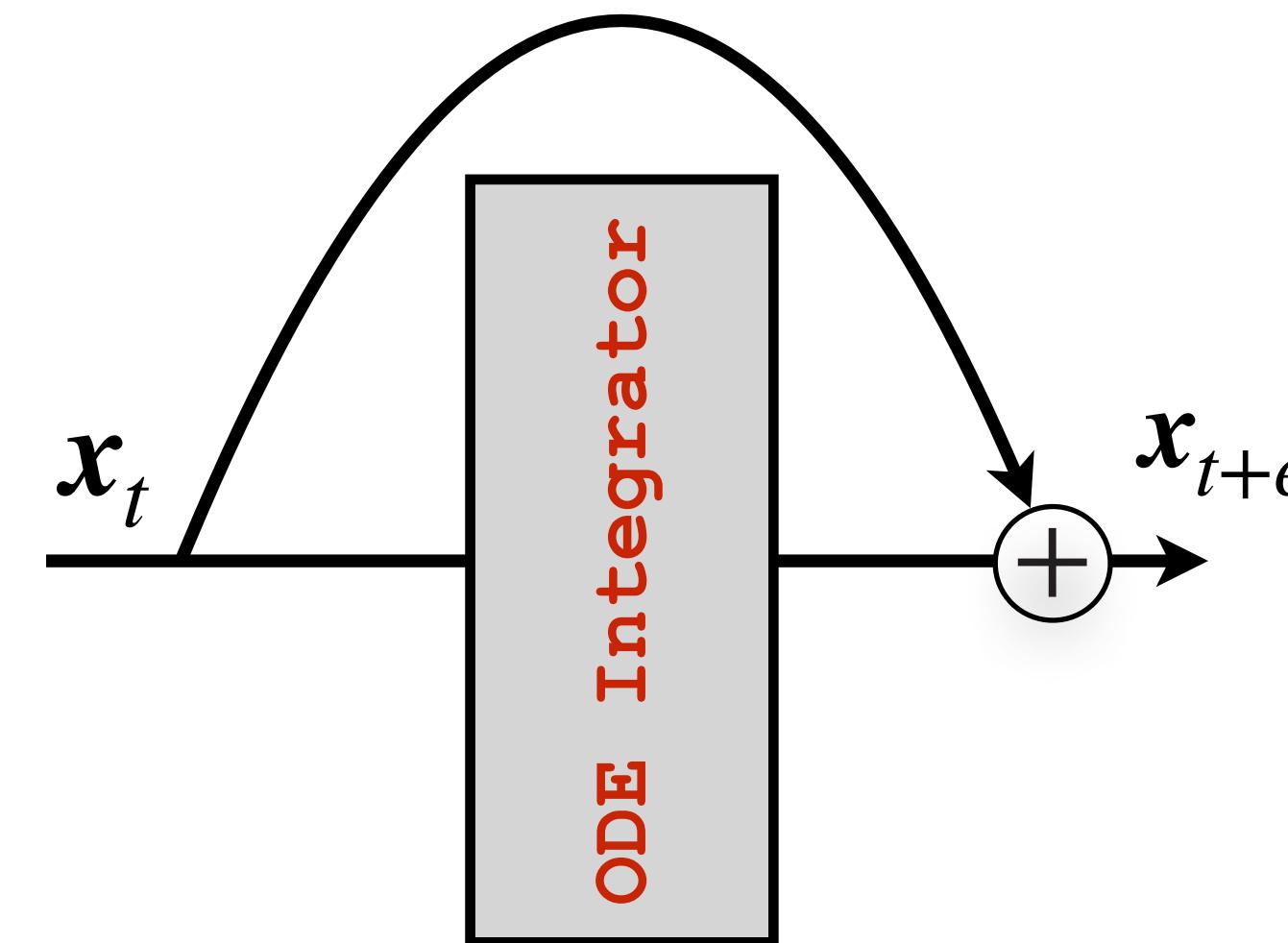
# Neural Ordinary Differential Equations

**Residual network**



$$x_{t+1} = x_t + f(x_t)$$

**ODE integration**



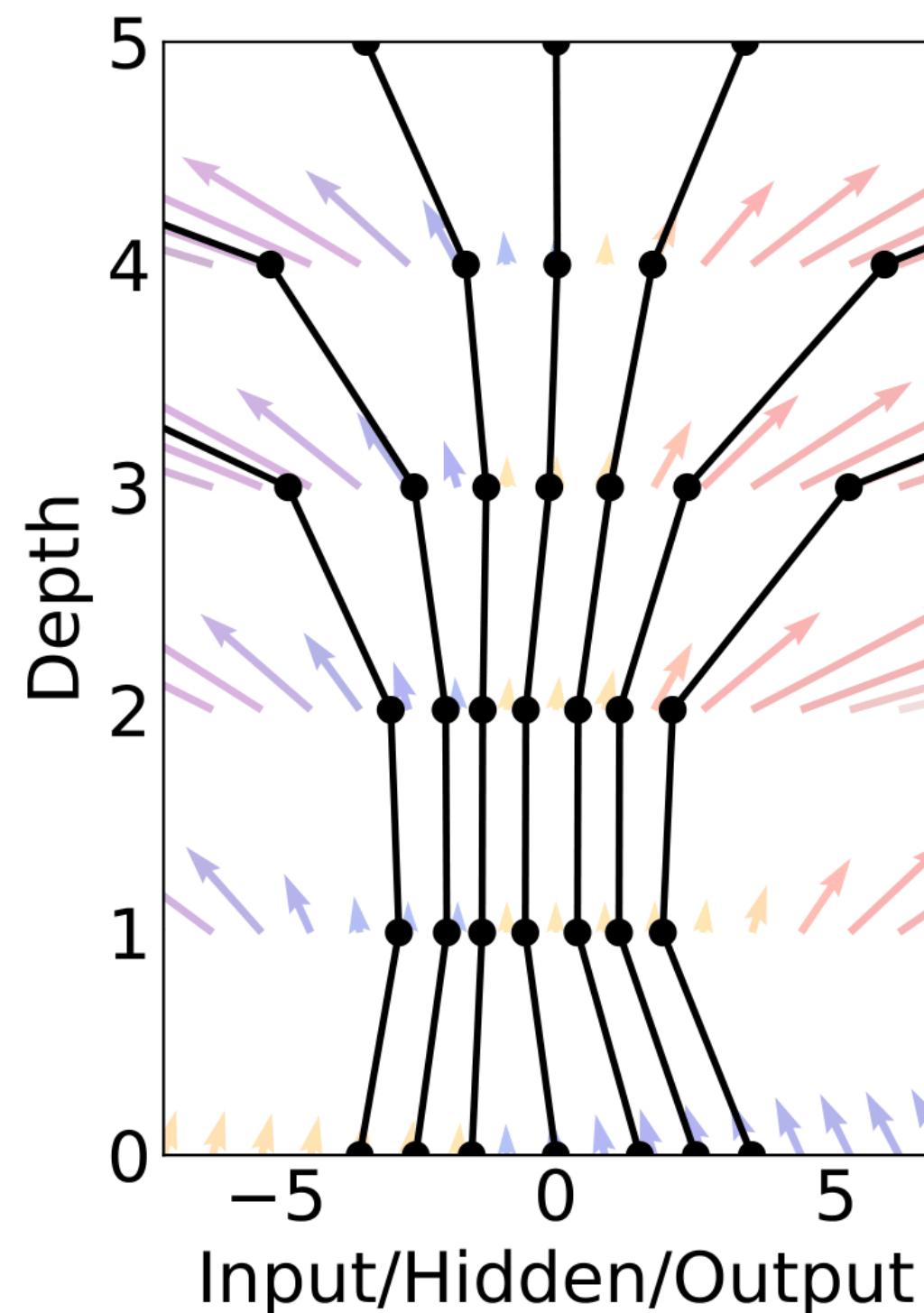
$$dx/dt = f(x)$$

Chen et al, 1806.07366

Harbor el al 1705.03341  
Lu et al 1710.10121,  
E Commun. Math. Stat 17'...

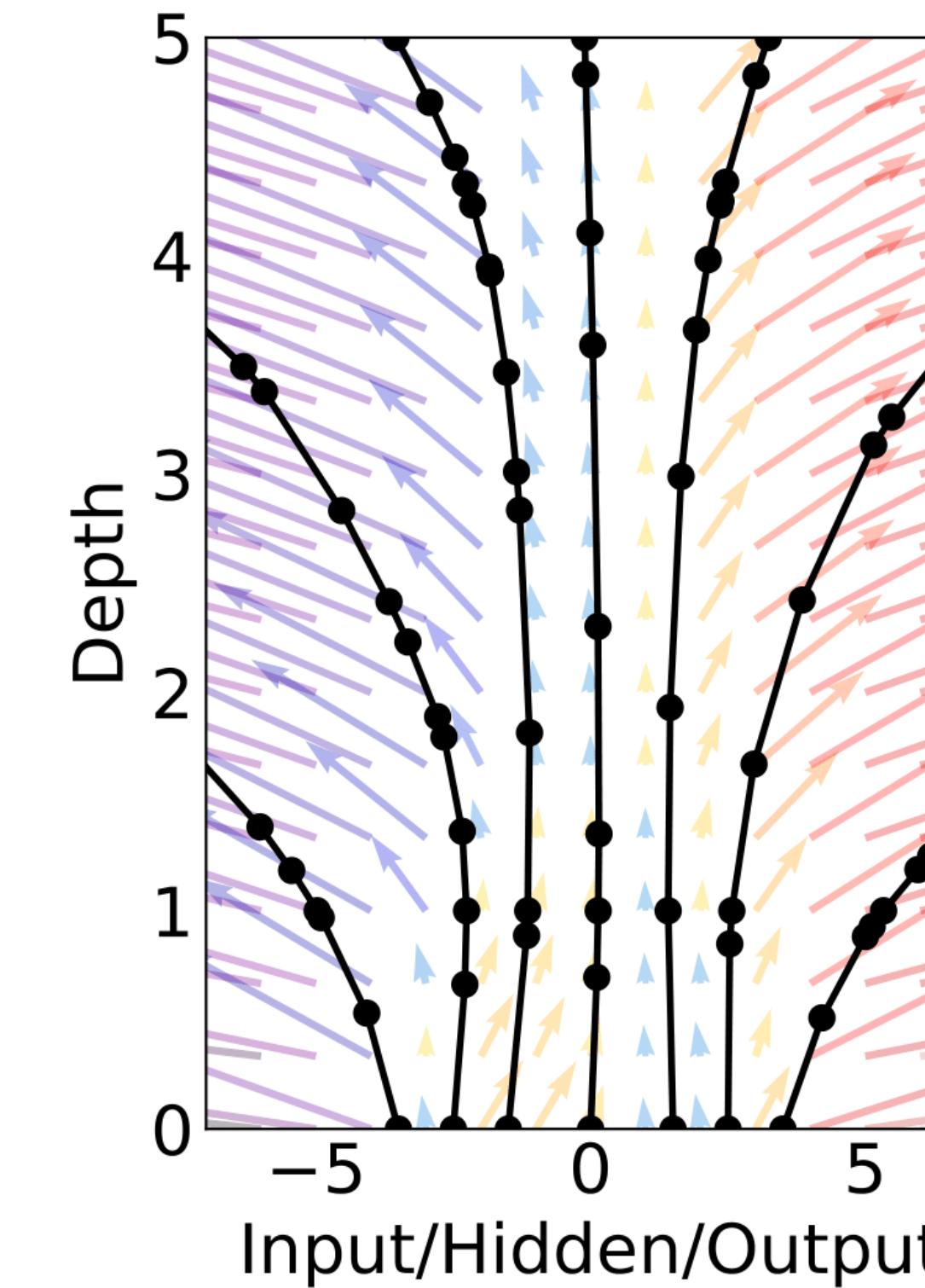
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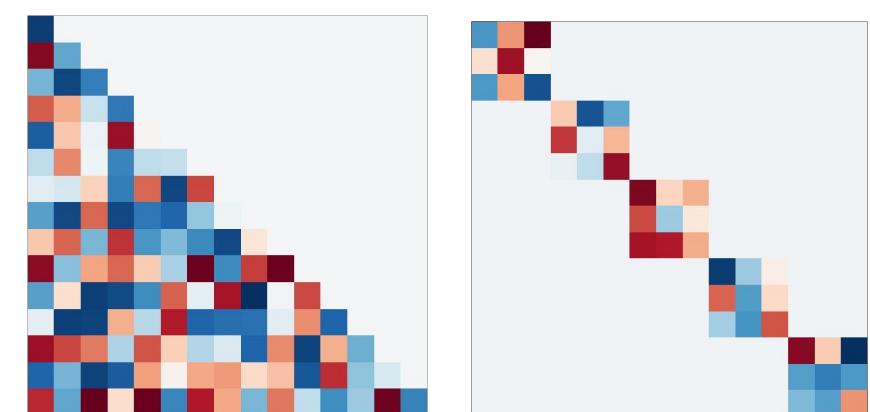
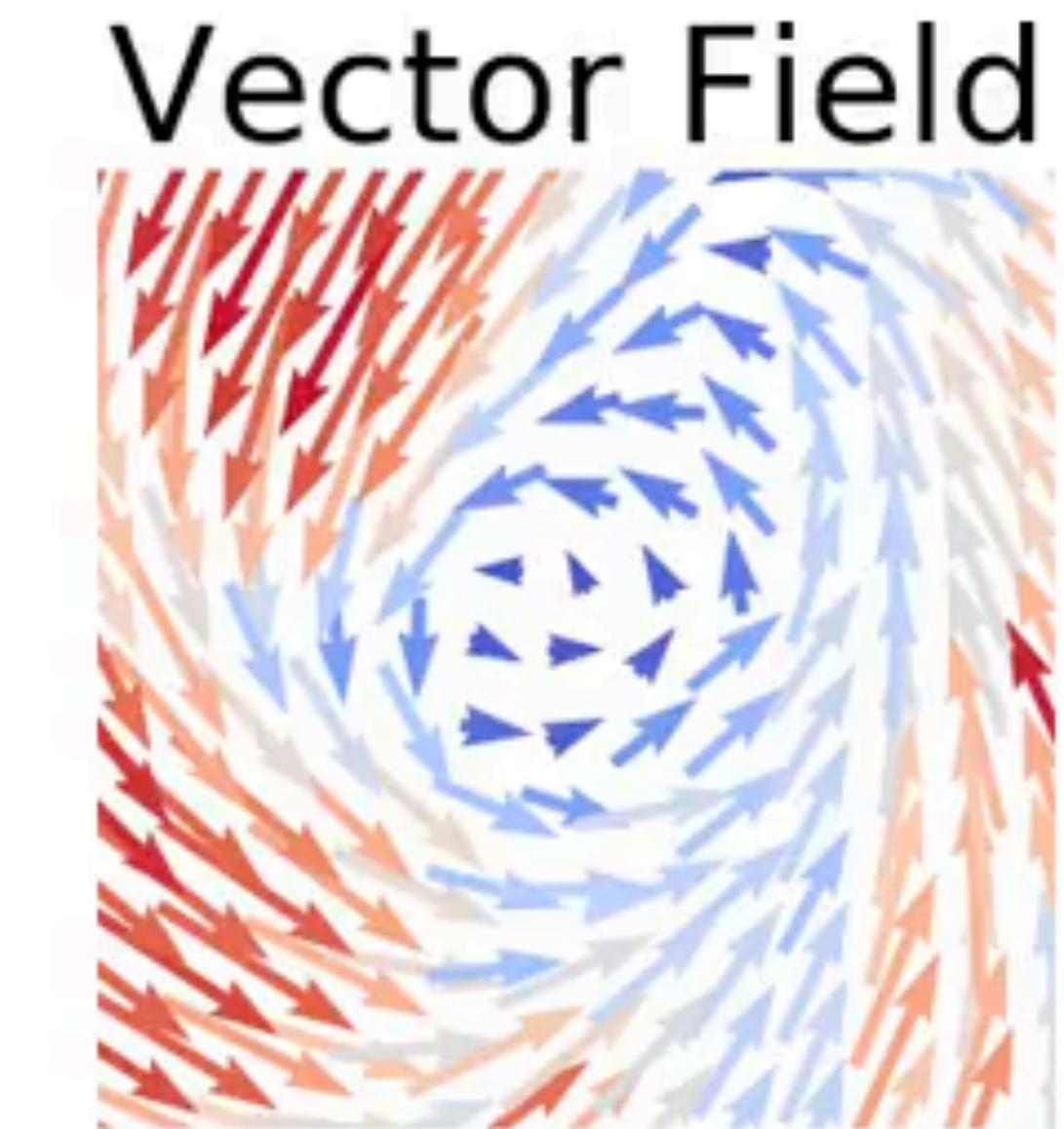
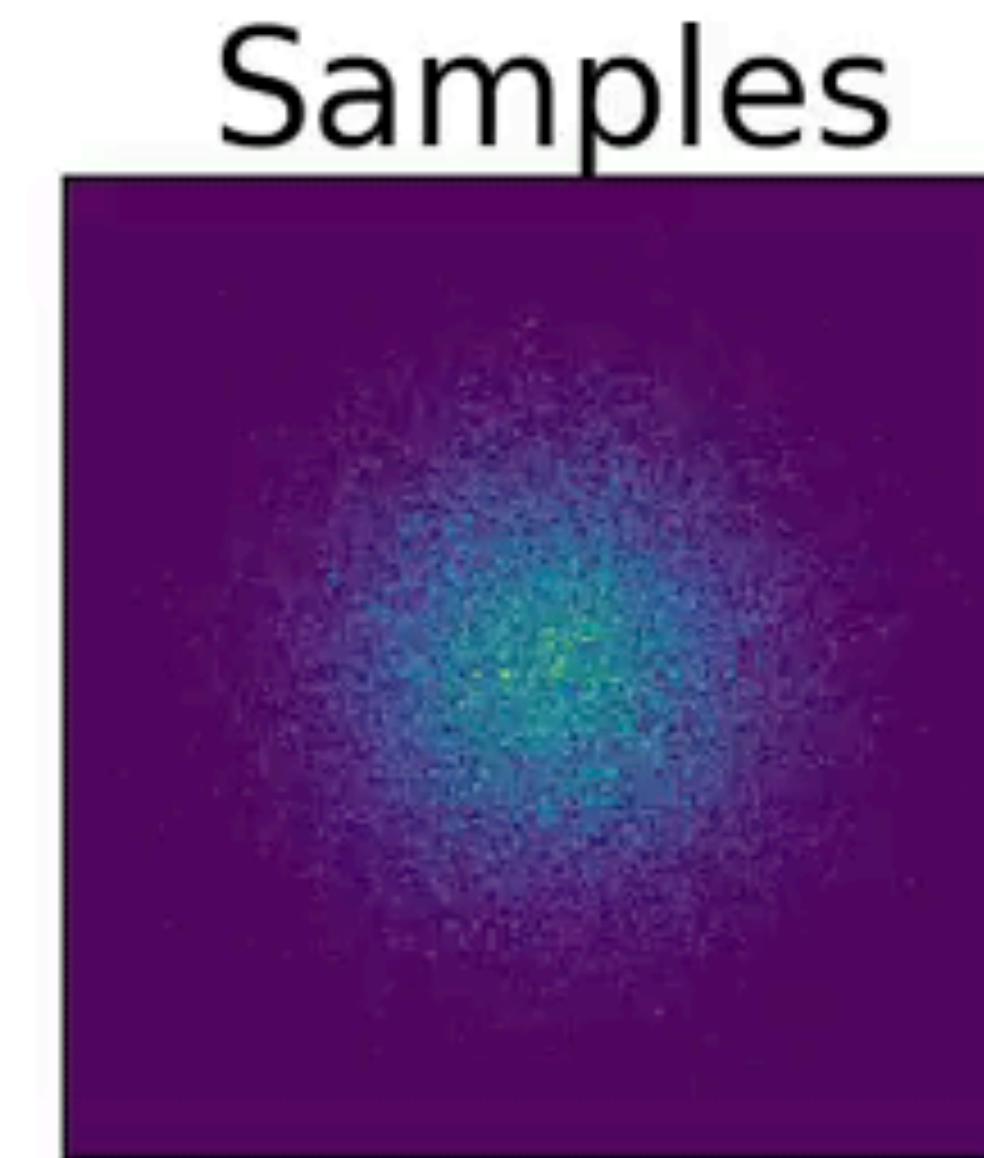
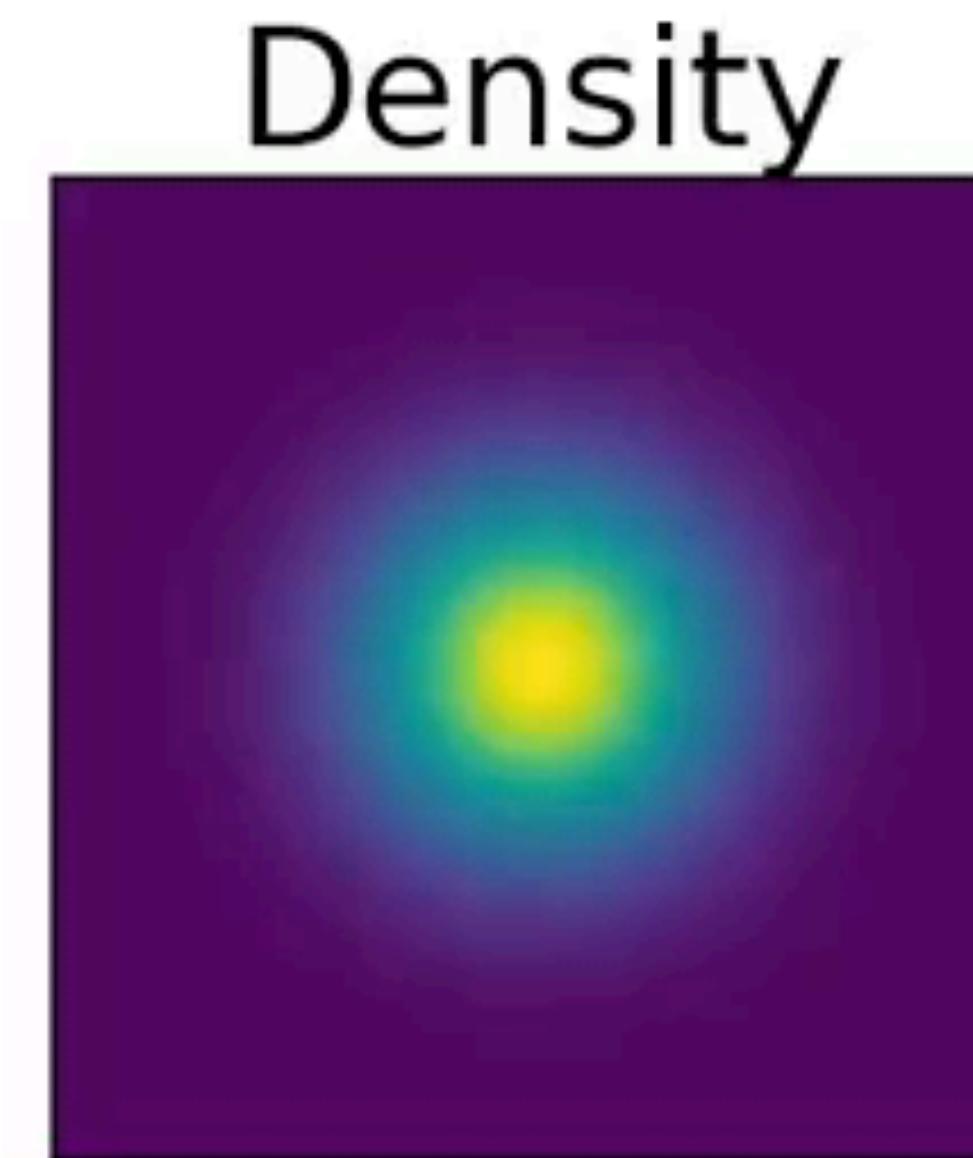
$$d\mathbf{x}/dt = f(\mathbf{x})$$

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Harbor el al 1705.03341  
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E Commun. Math. Stat 17'

# Neural Ordinary Differential Equations

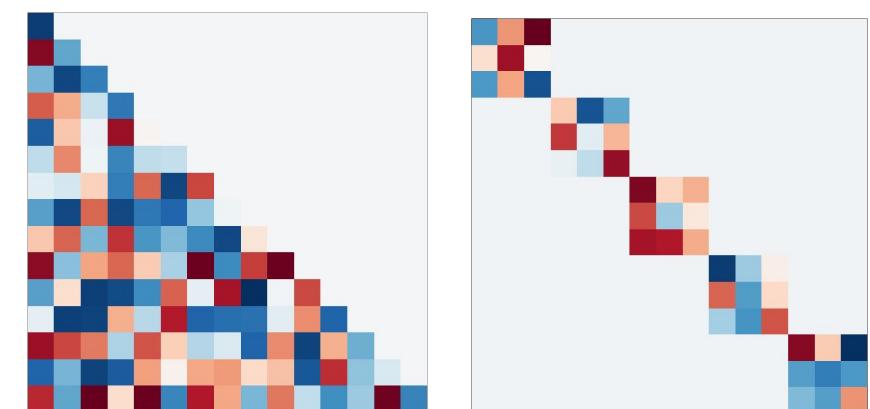
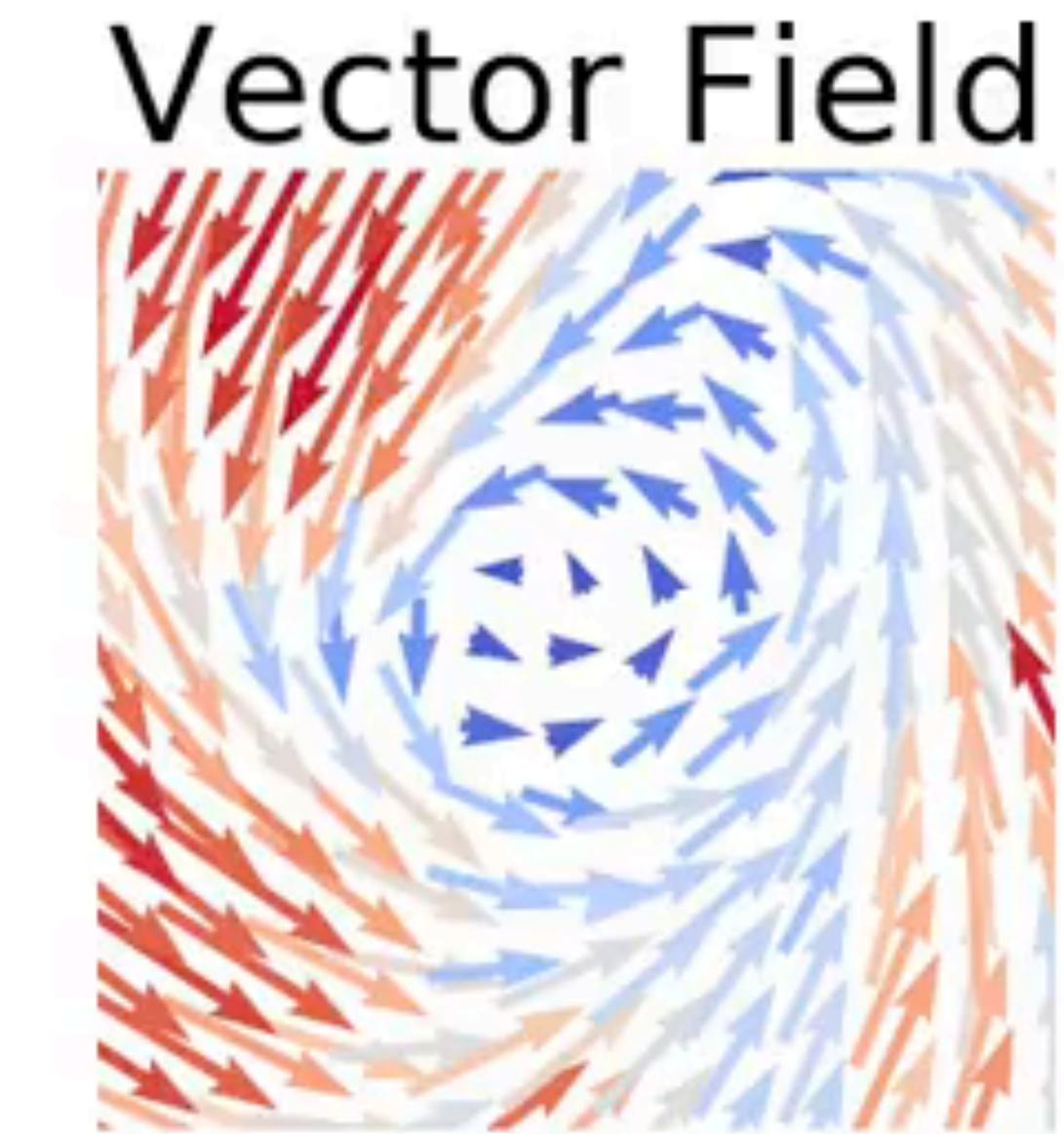
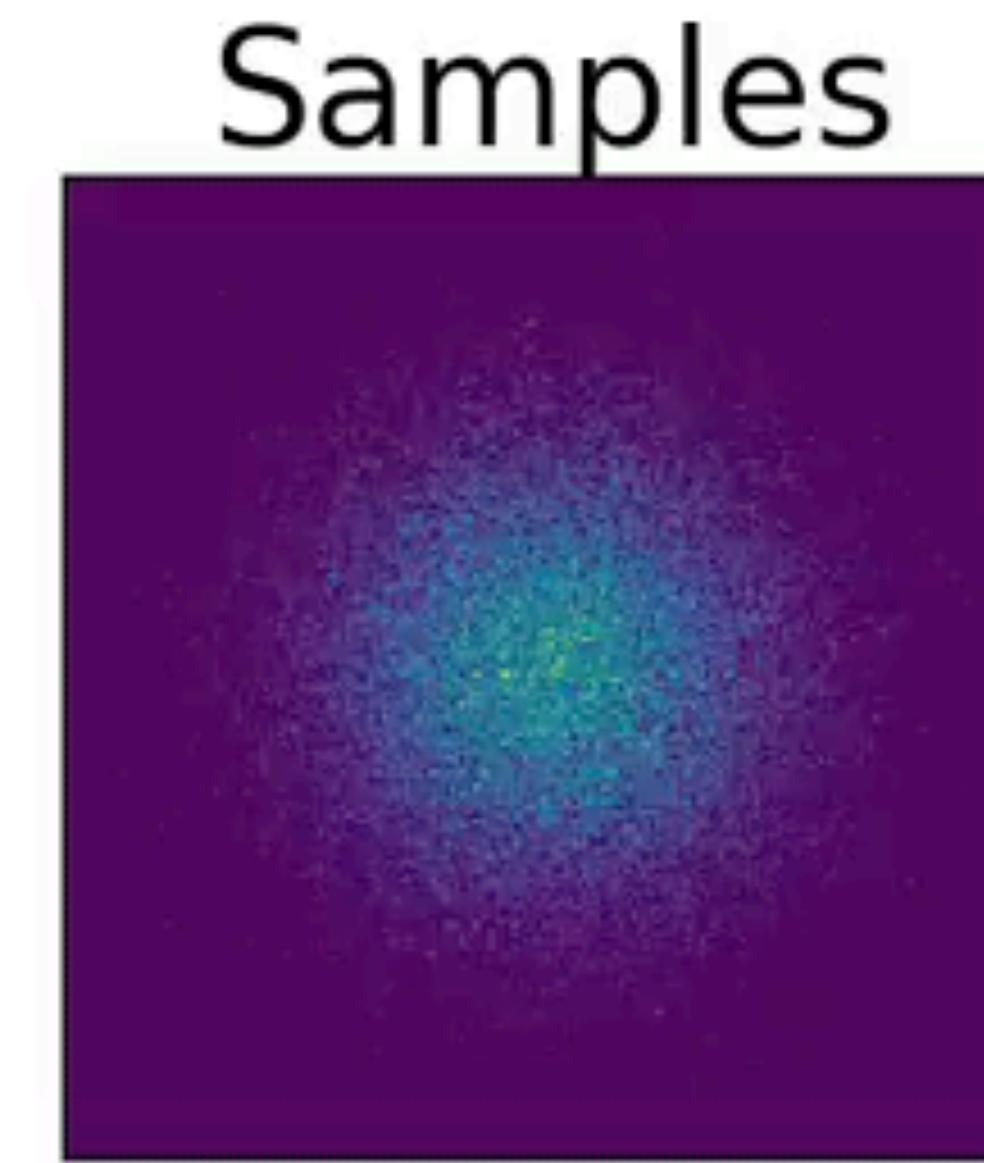
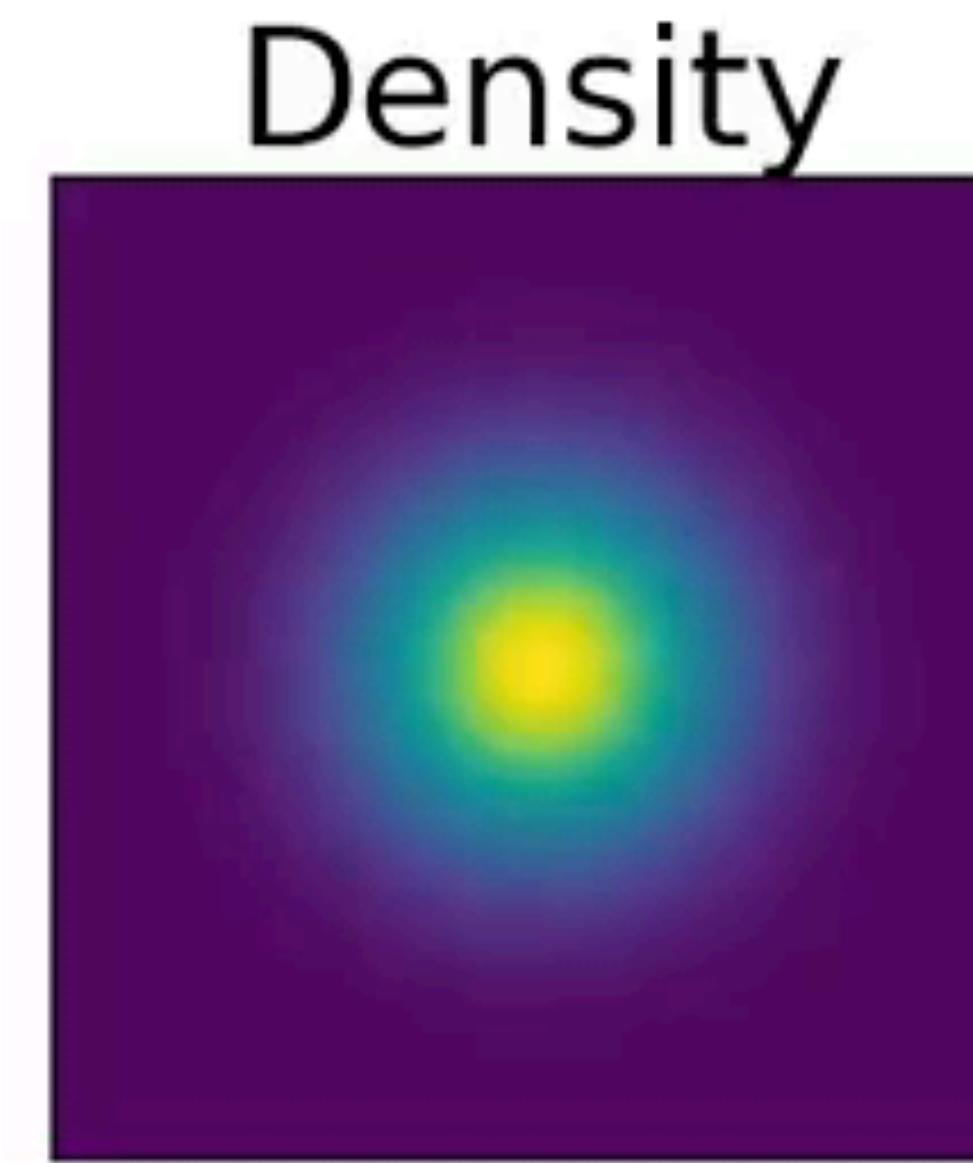
Chen et al, 1806.07366, Grathwohl et al 1810.01367



**Continuous normalizing flow have no structural constraints on the transformation Jacobian**

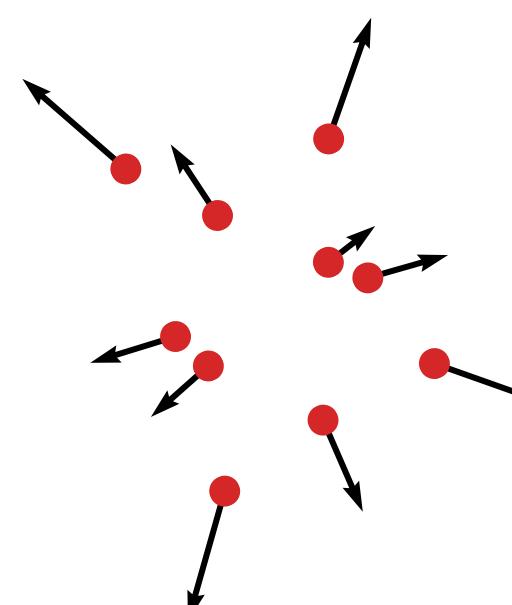
# Neural Ordinary Differential Equations

Chen et al, 1806.07366, Grathwohl et al 1810.01367



**Continuous normalizing flow have no structural constraints on the transformation Jacobian**

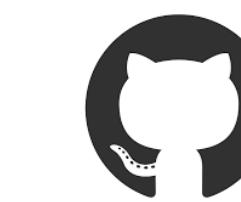
# Fluid physics behind flows

$$\frac{dx}{dt} = \nu$$


$$\frac{d \ln \rho(x, t)}{dt} = - \nabla \cdot \nu$$

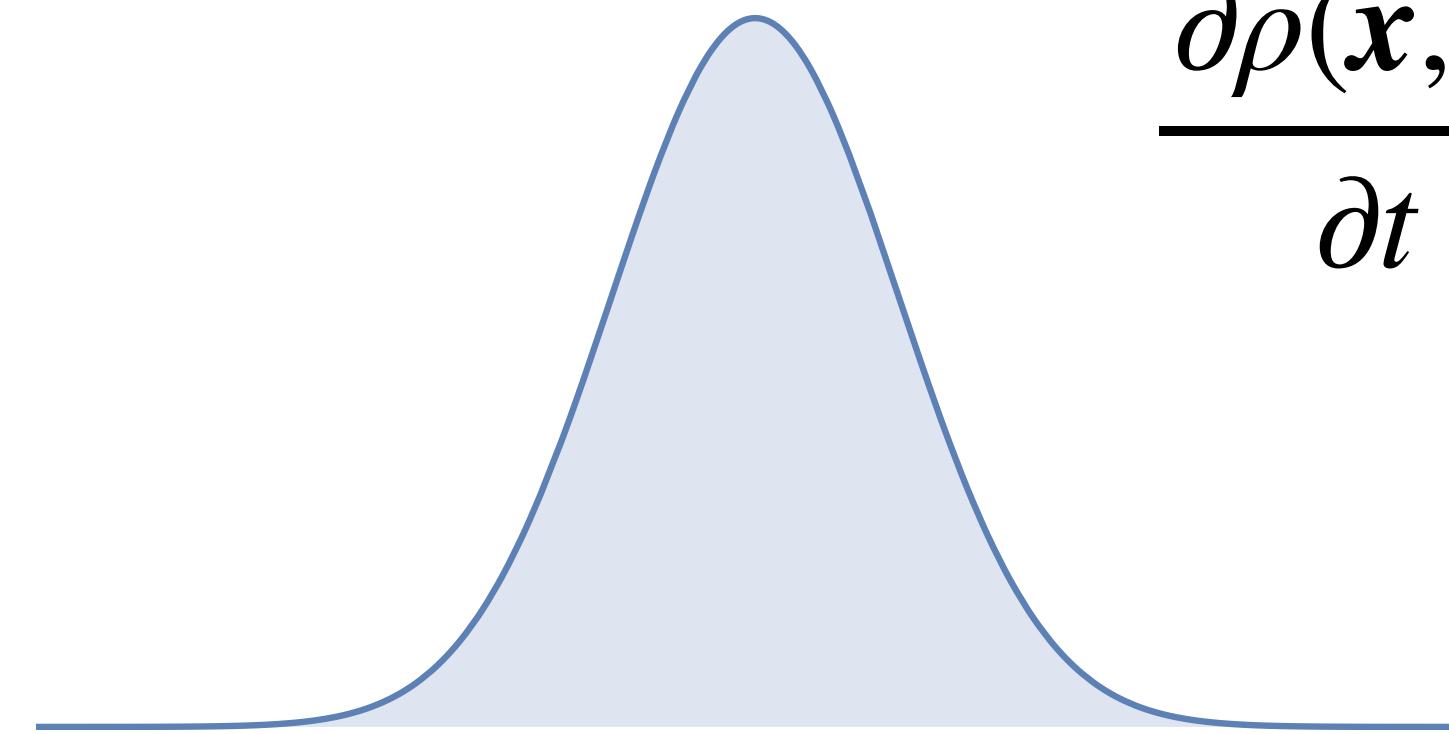
$$\frac{d}{dt} = \frac{\partial}{\partial t} + \nu \cdot \nabla$$

“material derivative”



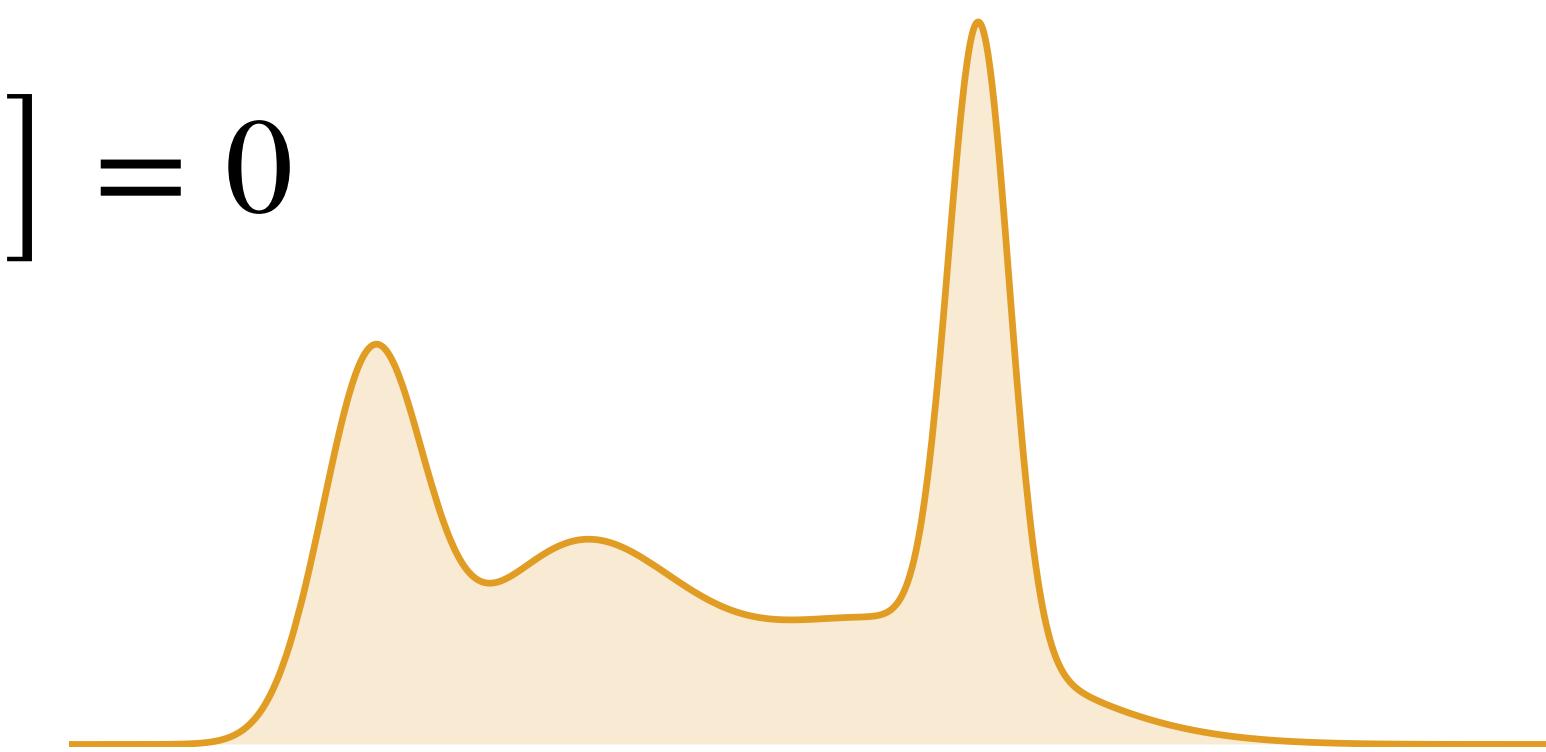
Zhang, E, LW 1809.10188

[wangleiphy/MongeAmpereFlow](https://github.com/wangleiphy/MongeAmpereFlow)



Simple density

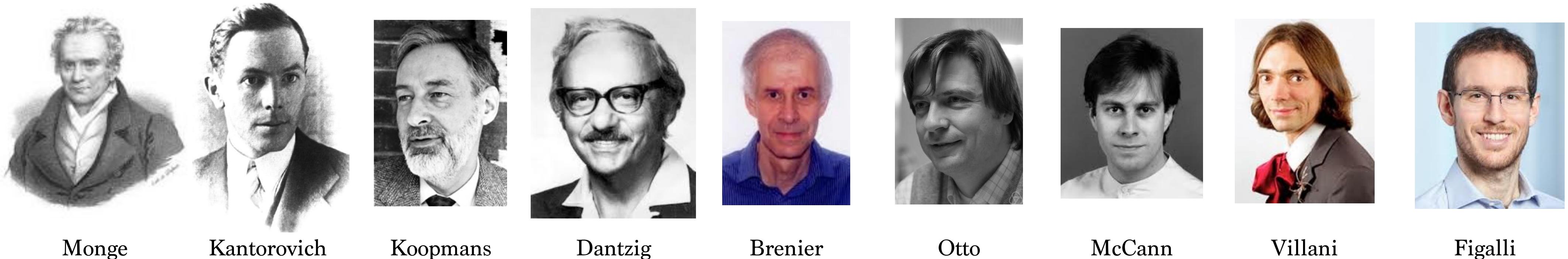
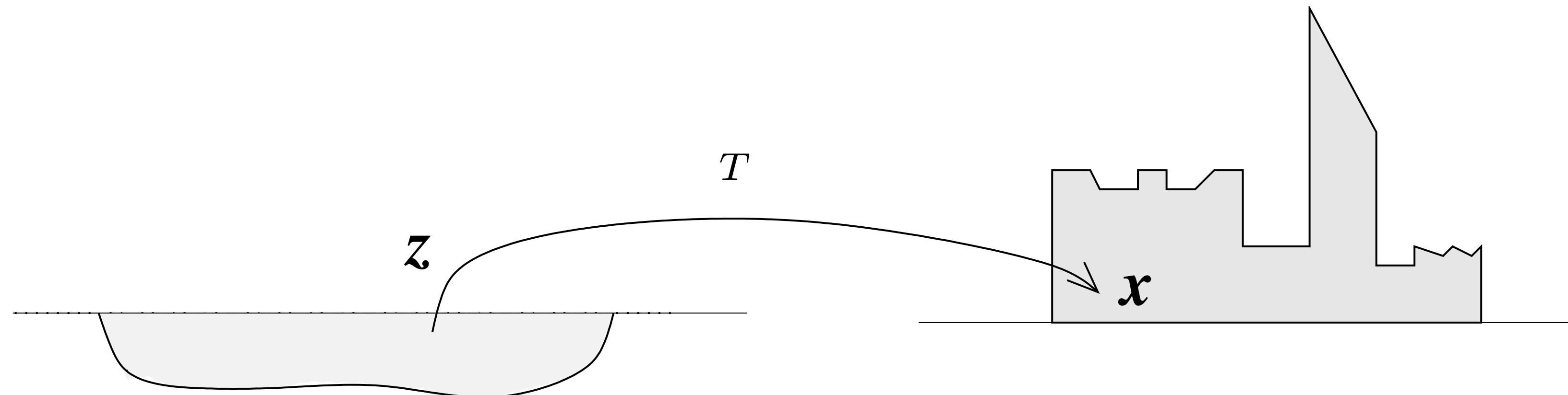
$$\frac{\partial \rho(x, t)}{\partial t} + \nabla \cdot [\rho(x, t) \nu] = 0$$



Complex density

# Optimal Transport Theory

**Monge problem (1781): How to transport earth with optimal cost ?**



Nobel Prize in Economics '75

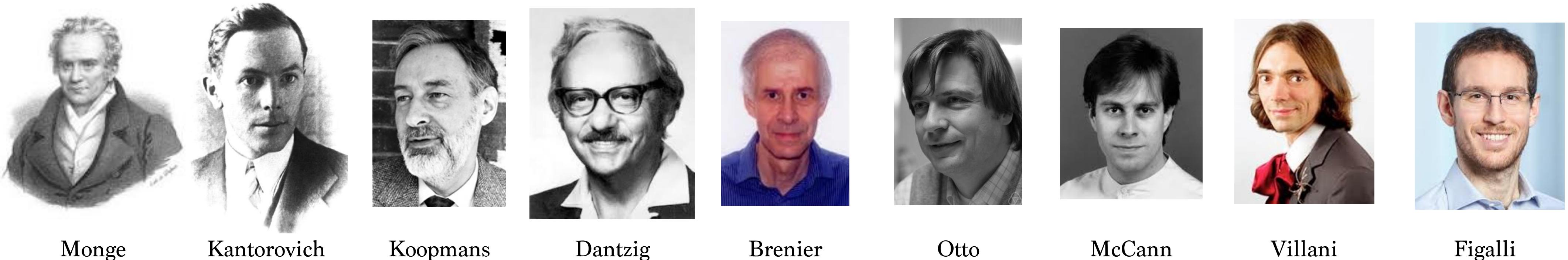
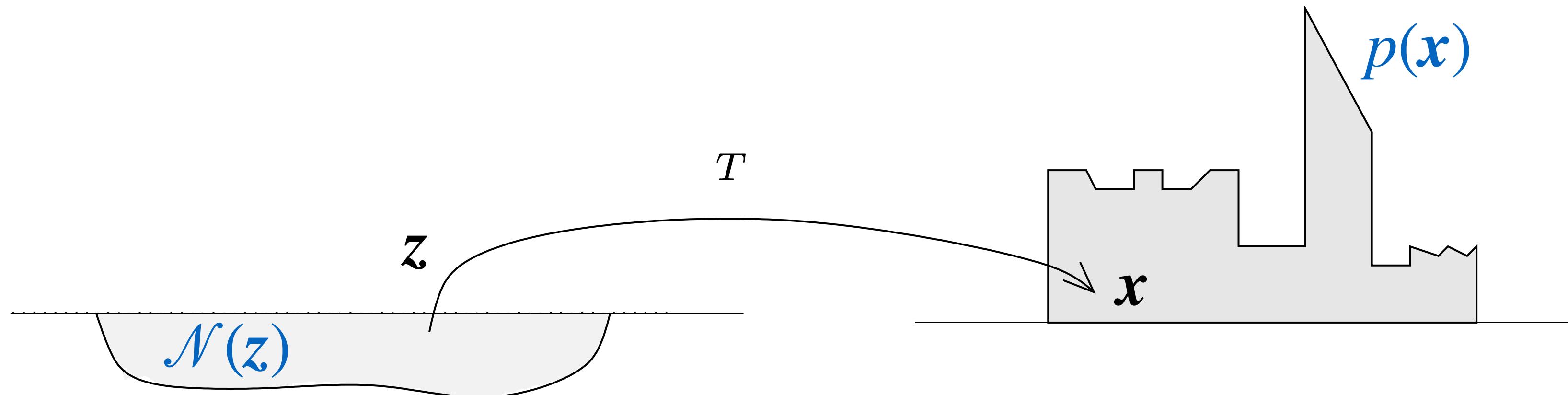
Fields Medal '10

Fields Medal '18

from Cuturi, Solomon NISP 2017 tutorial

# Optimal Transport Theory

**Monge problem (1781): How to transport earth with optimal cost ?**



Nobel Prize in Economics '75

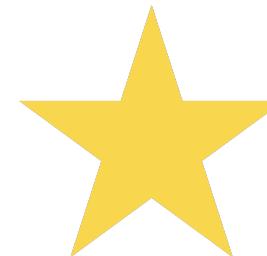
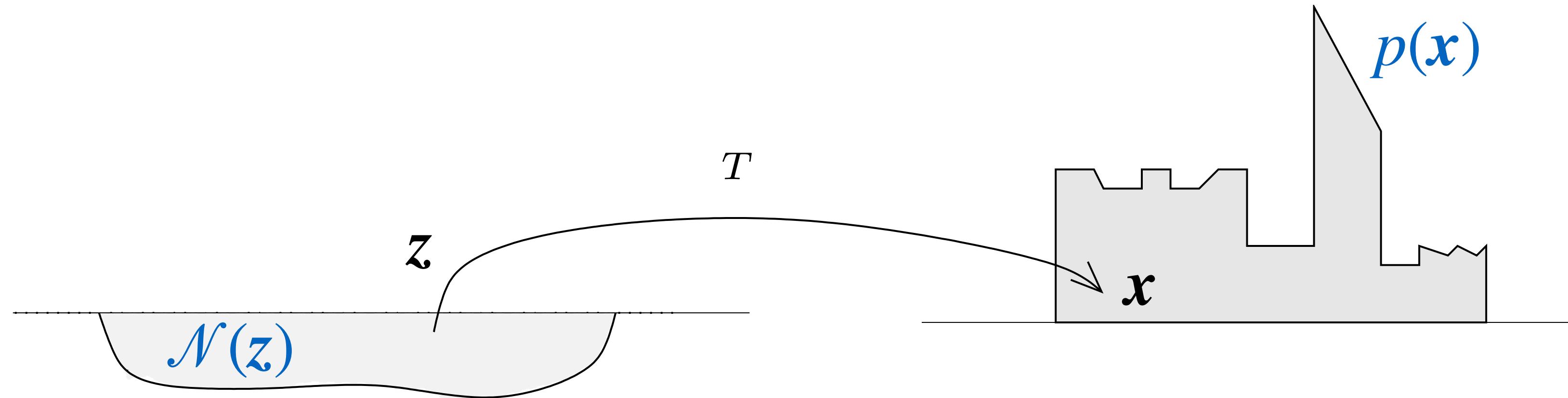
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# Optimal Transport Theory

**Monge problem (1781): How to transport earth with optimal cost ?**



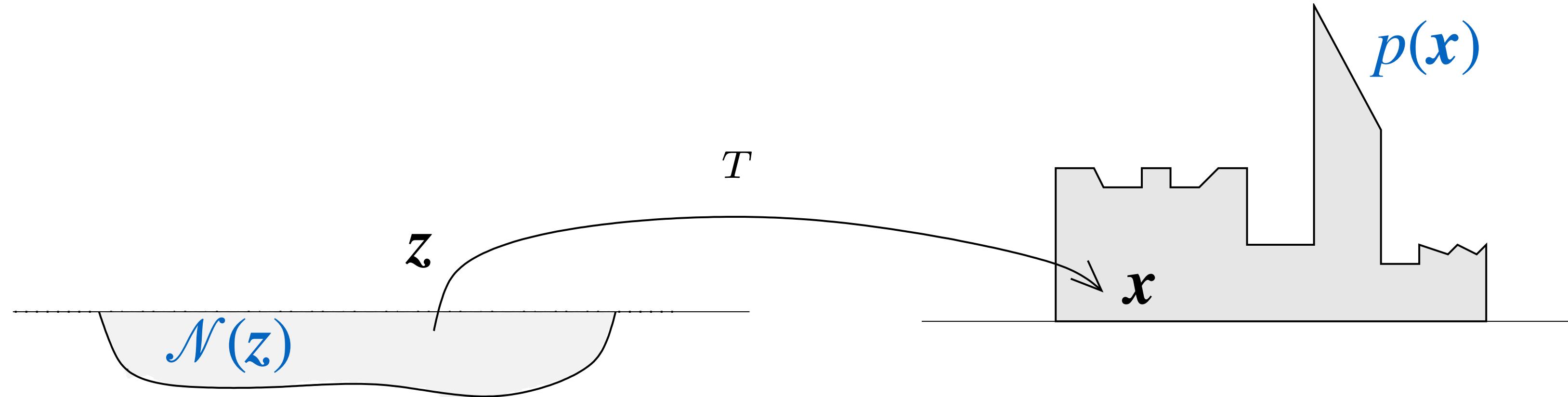
Brenier theorem (1991)

Under certain conditions  
the optimal map is

$$z \mapsto x = \nabla u(z)$$

# Optimal Transport Theory

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Brenier theorem (1991)

Under certain conditions  
the optimal map is

$$z \mapsto x = \nabla u(z)$$

Monge-Ampère Equation

$$\frac{\mathcal{N}(z)}{p(\nabla u(z))} = \det \left( \frac{\partial^2 u}{\partial z_i \partial z_j} \right)$$

# Monge-Ampère Flow

Zhang, E, LW 1809.10188



[wangleiphy/MongeAmpereFlow](https://github.com/wangleiphy/MongeAmpereFlow)

$$\frac{\partial \rho(x, t)}{\partial t} + \nabla \cdot [\rho(x, t) \nabla \varphi] = 0$$

- ① Drive the flow with an “irrotational” velocity field
- ② Impose symmetry to the scalar valued potential for symmetric generative model

$$\varphi(gx) = \varphi(x) \implies \rho(gx) = \rho(x)$$

# Hamiltonian dynamics: phase space flow

## Hamiltonian equations

$$\begin{cases} \dot{p} = -\frac{\partial H}{\partial q} \\ \dot{q} = +\frac{\partial H}{\partial p} \end{cases}$$

# Hamiltonian dynamics: phase space flow

**Hamiltonian equations**

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**Phase space variables**

$$x = (p, q)$$

**Symplectic metric**

$$J = \begin{pmatrix} & I \\ -I & \end{pmatrix}$$

# Hamiltonian dynamics: phase space flow

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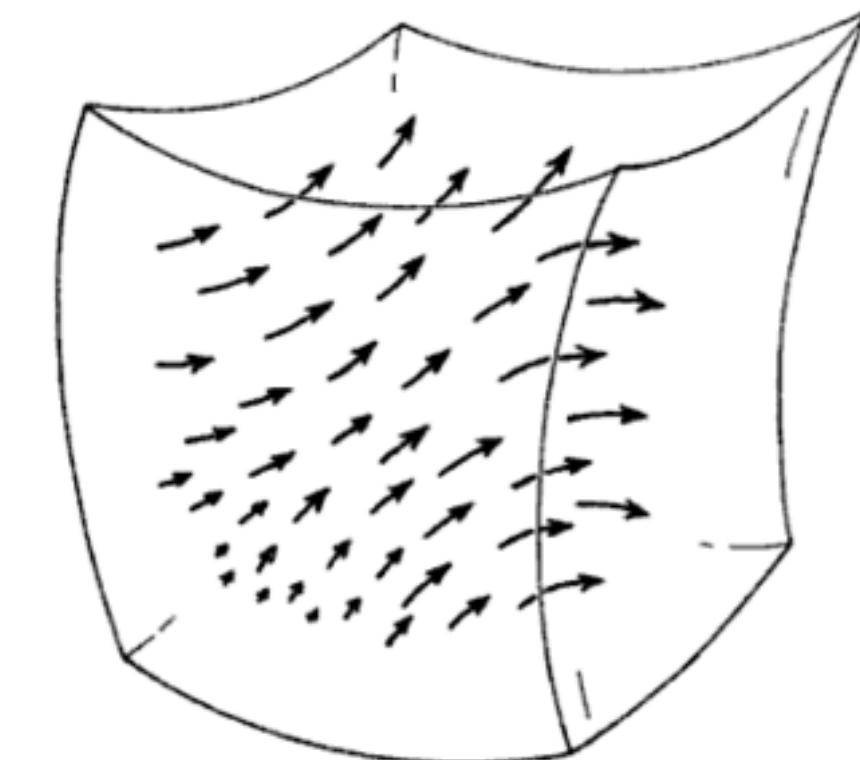
$$x = (p, q)$$

**Symplectic metric**

$$J = \begin{pmatrix} & I \\ -I & \end{pmatrix}$$

**Symplectic gradient flow**

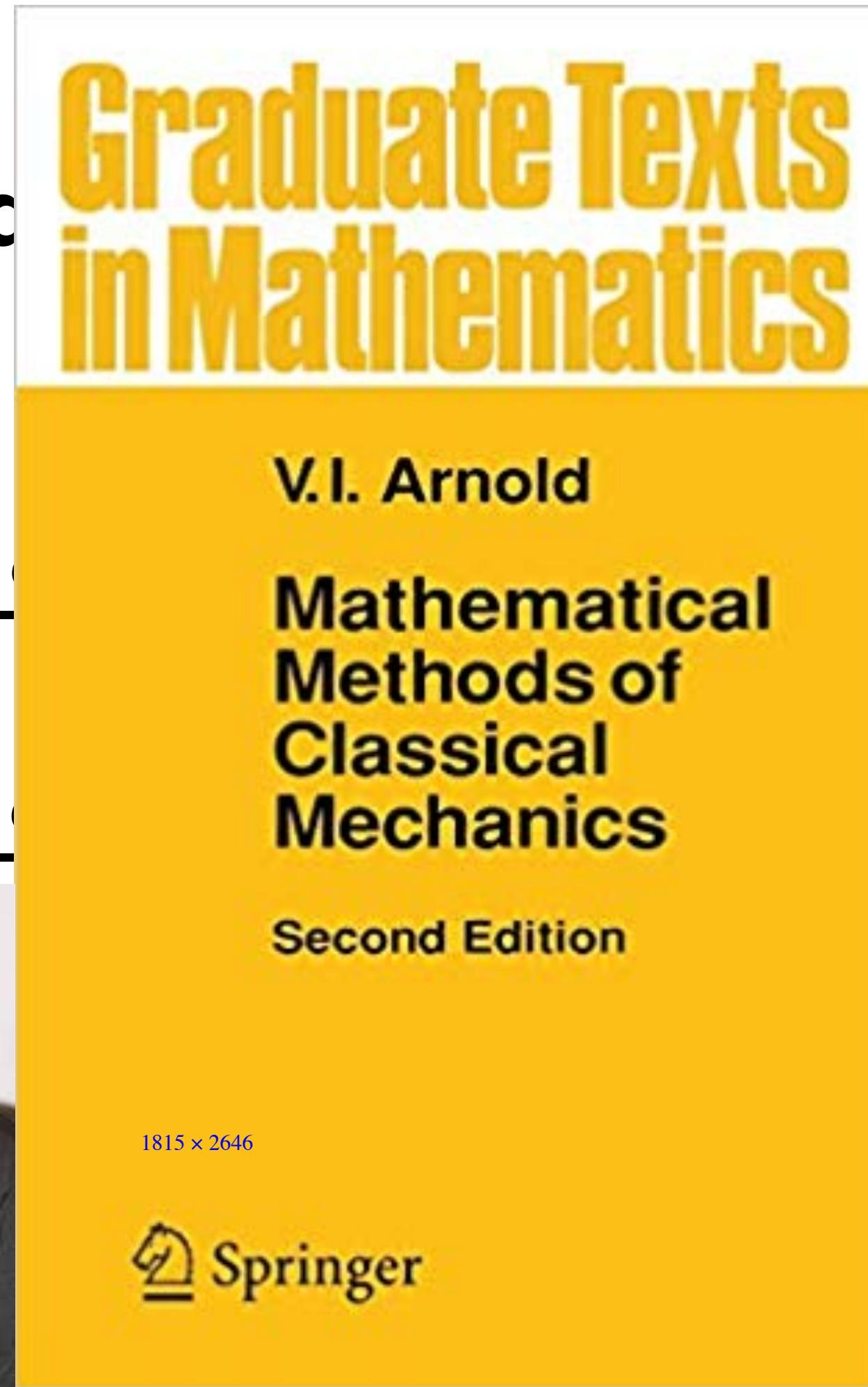
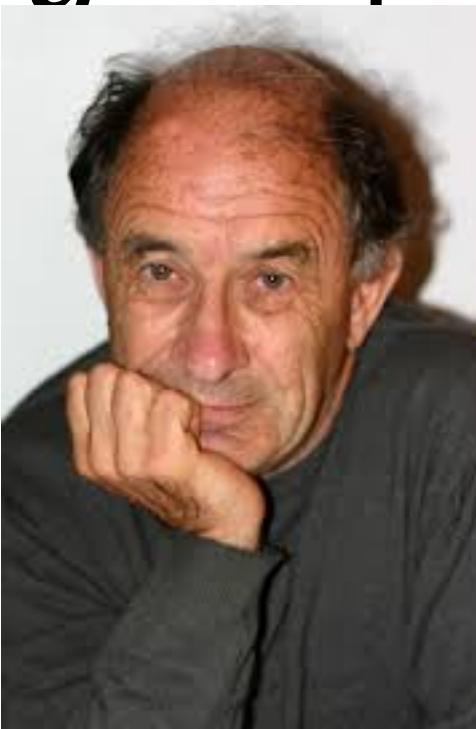
$$\dot{x} = \nabla_x H(x) J$$



# Hamiltonian dynamics: phase space flow

Hamiltonian eq

$$\begin{cases} \dot{p} = -\frac{\partial H}{\partial q} \\ \dot{q} = +\frac{\partial H}{\partial p} \end{cases}$$



pace va

$$= (p, q)$$

lectic m

$$\begin{pmatrix} I \\ -I \end{pmatrix}$$

Hamilton

Feng Kang Qin Mengzhao  
冯康 秦孟兆 著

浙江科学技术出版社

辛几何算法

哈密尔顿系统的

$$f^*\omega = \omega$$
$$\omega = \sum dp_i \wedge dq^i$$

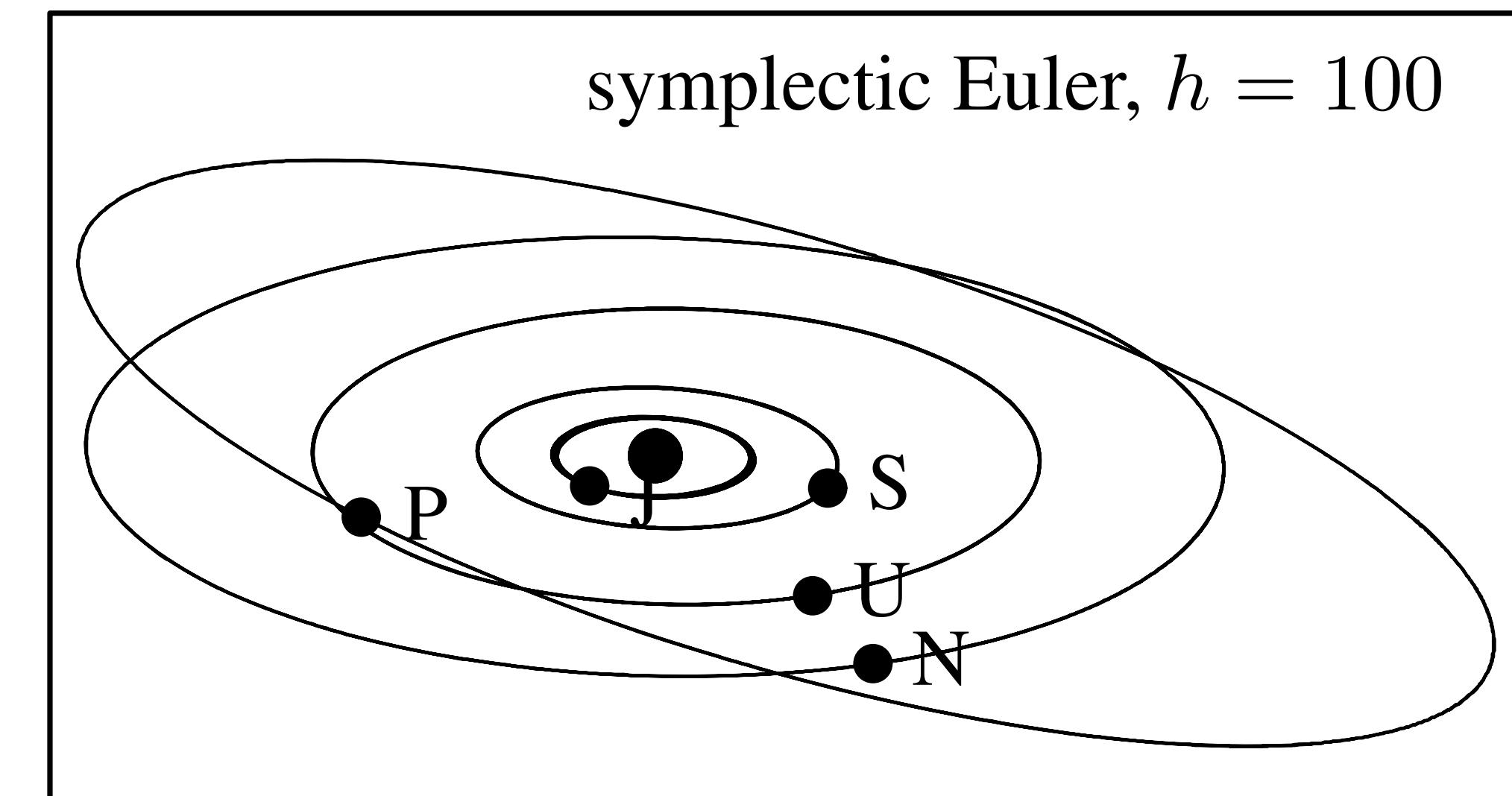
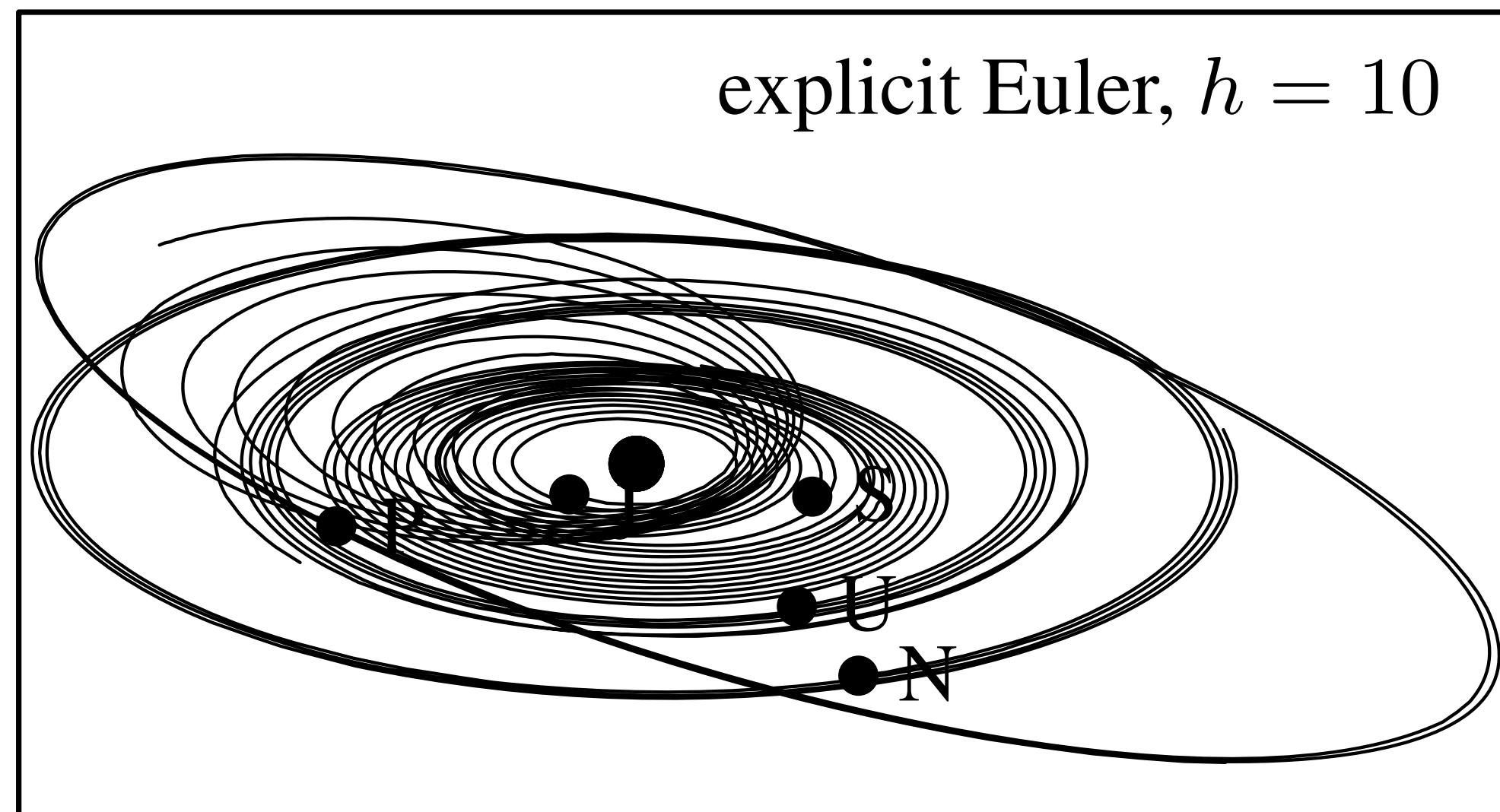
Symplectic Geometric  
Algorithms for  
Hamiltonian Systems



$$\nabla_x H(x) J$$

ic gradient flow

# Symplectic Integrators



# Canonical Transformations

$$x = (p, q) \quad \longleftrightarrow \quad z = (P, Q)$$

Change of variables

which satisfies

$$(\nabla_x z) J (\nabla_x z)^T = J$$

symplectic condition

# Canonical Transformations

$$x = (p, q) \quad \longleftrightarrow \quad z = (P, Q)$$

Change of variables

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symplectic condition

one has

$$\dot{z} = \nabla_z K(z) J \quad \text{where} \quad K(z) = H \circ x(z)$$

**Preserves Hamiltonian dynamics in the “latent phase space”**

# Canonical transformation for Moon-Earth-Sun 3-body problem

Gutzwiller, RMP, '98

<p><b>634</b></p> <p style="text-align: center;"><b>THÉORIE DU MOUVEMENT DE LA LUNE.</b></p> <div style="border-left: 1px solid black; padding-left: 10px;"> <math display="block">\begin{aligned} &amp; + \left( \frac{3}{8} e_i^1 - \frac{3}{4} \gamma_i^1 e_i^1 - \frac{3}{2} e_i^1 - \frac{411}{16} e_i^1 e^2 \right) \frac{n^2}{n_i^2} \\ &amp; + \left( \frac{219}{64} e_i^1 - \frac{99}{4} \gamma_i^1 e_i^1 - \frac{619}{32} e_i^1 - \frac{9843}{128} e_i^1 e^2 \right) \frac{n^3}{n_i^2} \\ &amp; \quad + \frac{189}{128} e_i^1 \frac{n^2}{n_i^2} - \frac{65337}{1024} e_i^1 \frac{n^4}{n_i^2} - \frac{5}{64} e_i^1 \frac{n^2}{n_i^2} \cdot \frac{a_1^2}{a^2} \Big] \cos \theta_i (t + e) \\ &amp; - \frac{99}{128} e_i^1 \frac{n^2}{n_i^2} \cos 2\theta_i (t + e), \end{aligned}</math> </div> <div style="border-left: 1px solid black; padding-left: 10px;"> <math display="block">\begin{aligned} \theta &amp;= \theta_i (t + e) \\ &amp; - \left[ \left( \frac{3}{4} - \frac{3}{2} \gamma_i^1 + \frac{3}{8} e_i^1 - \frac{15}{8} e^2 + \frac{3}{4} \gamma_i^1 + \frac{15}{4} \gamma_i^1 e^2 - \frac{171}{64} e_i^1 - \frac{15}{16} e_i^1 e^2 \right) \frac{n^2}{n_i^2} \right. \\ &amp; + \left( \frac{3}{8} - \frac{3}{4} \gamma_i^1 + \frac{21}{16} e_i^1 - \frac{411}{16} e^2 \right) \frac{n^3}{n_i^2} \\ &amp; \left. + \left( \frac{219}{64} - \frac{99}{4} \gamma_i^1 + \frac{1399}{128} e_i^1 - \frac{9843}{128} e^2 \right) \frac{n^4}{n_i^2} \right. \\ &amp; \quad \left. + \frac{189}{128} \frac{n^2}{n_i^2} - \frac{65337}{1024} \frac{n^4}{n_i^2} - \frac{5}{64} \frac{n^2}{n_i^2} \cdot \frac{a_1^2}{a^2} \right] \sin \theta_i (t + e) \\ &amp; + \left[ \left( \frac{9}{64} - \frac{9}{16} \gamma_i^1 - \frac{45}{128} e_i^1 - \frac{45}{64} e^2 \right) \frac{n^2}{n_i^2} + \frac{9}{64} \frac{n^3}{n_i^2} + \frac{675}{512} \frac{n^4}{n_i^2} \right] \sin 2\theta_i (t + e) \\ &amp; - \frac{9}{256} \frac{n^4}{n_i^2} \sin 3\theta_i (t + e). \end{aligned}</math> </div> <div style="border-left: 1px solid black; padding-left: 10px;"> <math display="block">\begin{aligned} a &amp;= a_i \left\{ 1 + \left[ \left( \frac{3}{2} e_i^1 - 3\gamma_i^1 e_i^1 - \frac{15}{4} e_i^1 - \frac{15}{4} e_i^1 e^2 + \frac{3}{2} \gamma_i^1 e_i^1 + \frac{15}{2} \gamma_i^1 e_i^1 \right. \right. \right. \\ &amp; \quad \left. \left. \left. + \frac{15}{2} \gamma_i^1 e_i^1 e^2 + \frac{101}{32} e_i^1 e^2 + \frac{75}{8} e_i^1 e^2 \right) \frac{n^2}{n_i^2} \right. \\ &amp; \quad \left. + \left( \frac{3}{4} e_i^1 - \frac{3}{2} \gamma_i^1 e_i^1 - \frac{15}{8} e_i^1 - \frac{411}{8} e_i^1 e^2 \right) \frac{n^3}{n_i^2} \right. \\ &amp; \quad \left. + \left( \frac{219}{32} e_i^1 - \frac{99}{2} \gamma_i^1 e_i^1 - \frac{1819}{64} e_i^1 - \frac{9843}{64} e_i^1 e^2 \right) \frac{n^4}{n_i^2} \right. \\ &amp; \quad \left. + \frac{189}{64} e_i^1 \frac{n^2}{n_i^2} - \frac{27349}{512} e_i^1 \frac{n^4}{n_i^2} - \frac{5}{32} e_i^1 \frac{n^2}{n_i^2} \cdot \frac{a_1^2}{a^2} \right] \cos \theta_i (t + e) \\ &amp; \quad \left. - \frac{9}{16} e_i^1 \frac{n^2}{n_i^2} \cos 2\theta_i (t + e) \right\}, \end{aligned}</math> </div> <div style="border-left: 1px solid black; padding-left: 10px;"> <math display="block">\begin{aligned} \gamma^1 &amp;= \gamma_i^1 - \left[ \left( \frac{3}{8} \gamma_i^1 e_i^1 - \frac{3}{4} \gamma_i^1 e_i^1 - \frac{3}{4} \gamma_i^1 e_i^1 - \frac{15}{16} \gamma_i^1 e_i^1 e^2 \right) \frac{n^2}{n_i^2} \right. \\ &amp; \quad \left. + \frac{3}{16} \gamma_i^1 e_i^1 \frac{n^3}{n_i^2} + \frac{219}{128} \gamma_i^1 e_i^1 \frac{n^4}{n_i^2} \right] \cos \theta_i (t + e). \end{aligned}</math> </div>	<p><b>640</b></p> <p style="text-align: center;"><b>THÉORIE DU MOUVEMENT DE LA LUNE.</b></p> <div style="border-left: 1px solid black; padding-left: 10px;"> <math display="block">\begin{aligned} &amp; + \left( \frac{13}{64} + \frac{187}{32} \gamma^1 - \frac{237}{128} e^2 + \frac{195}{128} e^3 - \frac{1389}{32} \gamma^1 - \frac{599}{64} \gamma^1 e^1 + \frac{2805}{64} \gamma^1 e^2 \right. \\ &amp; \quad \left. - \frac{103173}{1024} e^1 - \frac{3105}{256} e^3 e^2 \right) \frac{n^2}{n^2} \\ &amp; + \left( \frac{79}{16} + \frac{55}{48} \gamma^1 - \frac{1063}{48} e^2 + \frac{2133}{32} e^3 \right) \frac{n^3}{n^2} + \left( \frac{153}{8} + \frac{345}{96} \gamma^1 - \frac{73159}{768} e^2 + \frac{249085}{512} e^3 \right) \frac{n^4}{n^2} \\ &amp; \quad + \frac{22441}{288} \frac{n^2}{n^2} + \frac{99916415}{442368} \frac{n^4}{n^2} + \frac{4431}{2048} \frac{n^2}{n^2} \cdot \frac{a^2}{a^2}. \end{aligned}</math> </div>
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De ces valeurs de L, G, H, on déduit

$$\frac{dL}{dt} = \frac{1}{an} \left\{ 1 + \left( \frac{1991}{32} - \frac{1629}{8} \gamma^1 + \frac{34985}{128} e^2 + \frac{28635}{64} e^3 \right) \frac{n^2}{n^2} \right. \\ \quad \left. + \left( \frac{415}{2} - \frac{2745}{4} \gamma^1 + \frac{31449}{16} e^2 + \frac{43299}{16} e^3 \right) \frac{n^3}{n^2} + \frac{61185}{64} \frac{n^4}{n^2} + \frac{1532167}{576} \frac{n^2}{n^2} \right\},$$

$$\frac{dG}{dt} = - \frac{1}{an} \left\{ \left( \frac{527}{8} - \frac{3633}{16} \gamma^1 - \frac{9991}{128} e^2 + 480 e^3 \right) \frac{n^2}{n^2} \right. \\ \quad \left. + \left( \frac{2757}{8} - \frac{2493}{2} \gamma^1 - \frac{2161}{16} e^2 + \frac{36459}{8} e^3 \right) \frac{n^3}{n^2} + \frac{104117}{64} \frac{n^4}{n^2} + \frac{277537}{48} \frac{n^2}{n^2} \right\},$$

$$\frac{dH}{dt} = - \frac{1}{an} \left\{ \left( \frac{15}{16} + \frac{15}{16} \gamma^1 - \frac{1809}{32} e^2 + \frac{225}{32} e^3 \right) \frac{n^2}{n^2} \right. \\ \quad \left. + \left( \frac{167}{8} - 66 \gamma^1 - \frac{265}{8} e^2 + \frac{4509}{16} e^3 \right) \frac{n^3}{n^2} + \frac{895}{16} \frac{n^4}{n^2} + \frac{176531}{576} \frac{n^2}{n^2} \right\},$$

$$\frac{dL}{dt} = \frac{1}{a^2 n e} \left\{ 1 - e^2 + \left( \frac{1991}{64} - \frac{1113}{16} \gamma^1 - \frac{40571}{128} e^2 + \frac{28065}{128} e^3 \right) \frac{n^2}{n^2} + \frac{3343}{24} \frac{n^4}{n^2} + \frac{62483}{96} \frac{n^2}{n^2} \right\},$$

$$\frac{dG}{dt} = - \frac{1}{a^2 n e} \left\{ 1 - \frac{1}{2} e^2 - \frac{1}{8} e^4 - \frac{1}{16} e^6 \right. \\ \quad \left. + \left( \frac{1991}{64} - \frac{1113}{16} \gamma^1 - \frac{3831}{8} e^2 + \frac{28065}{128} e^3 \right) \frac{n^2}{n^2} + \frac{3343}{24} \frac{n^4}{n^2} + \frac{62483}{96} \frac{n^2}{n^2} \right\},$$

$$\frac{dH}{dt} = \frac{1}{a^2 n e} \cdot \frac{141}{8} e^2 \frac{n^2}{n^2},$$

$$\frac{d\gamma^1}{dt} = \frac{1}{a^2 n^2} \cdot \frac{183}{32} \gamma^1 \frac{n^2}{n^2},$$


Charles Delaunay



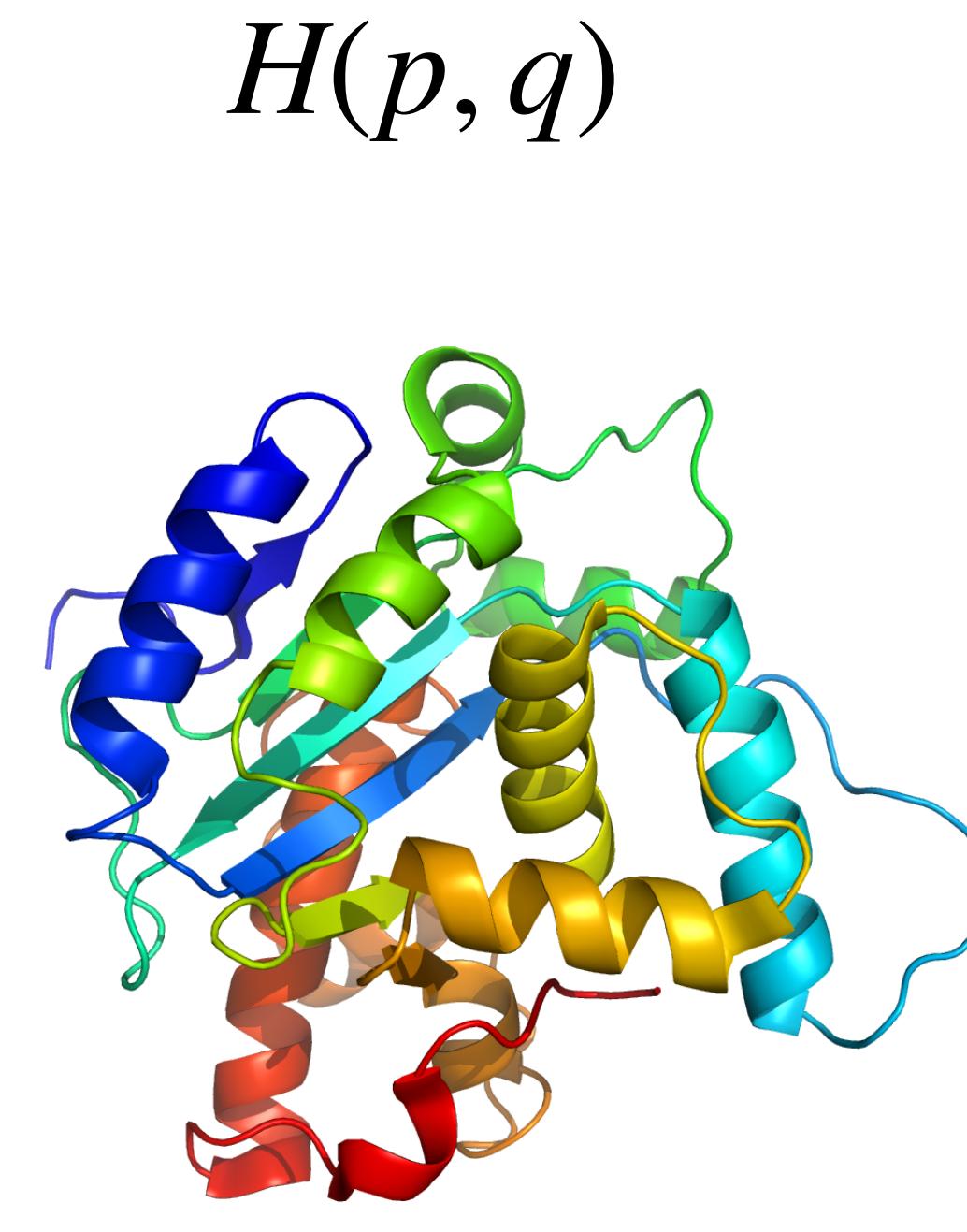
More than 1800 pages of this, ~20 years of efforts (1846-1867)

# Neural Canonical Transformations

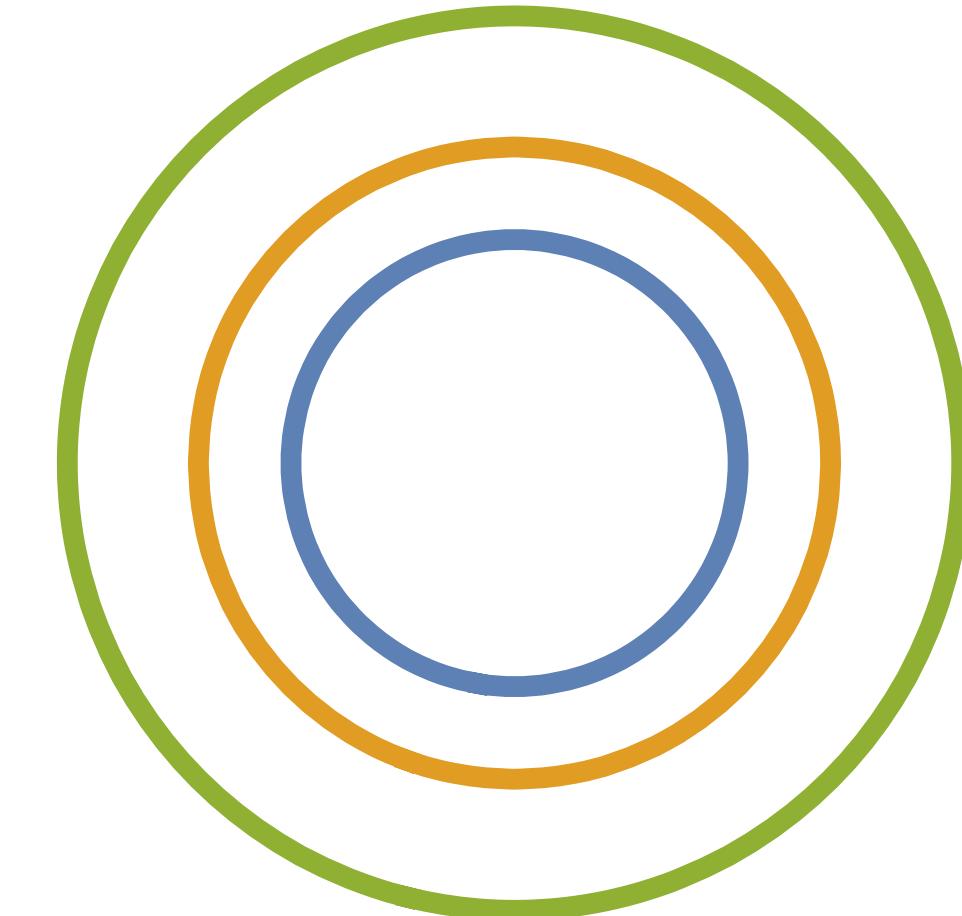
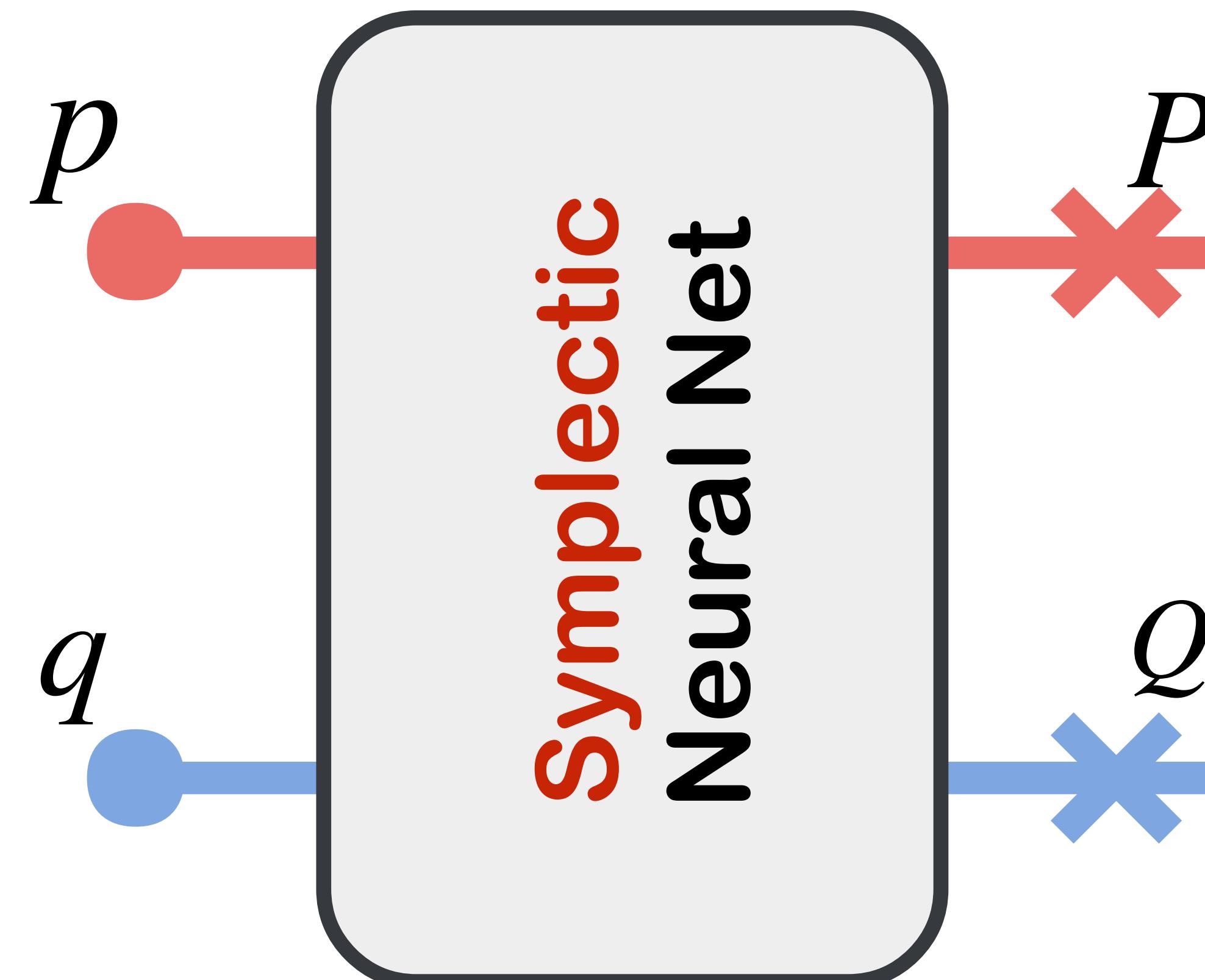
Li, Dong, Zhang, LW, PRX '20



[li012589/neuralCT](https://github.com/li012589/neuralCT)



physical space

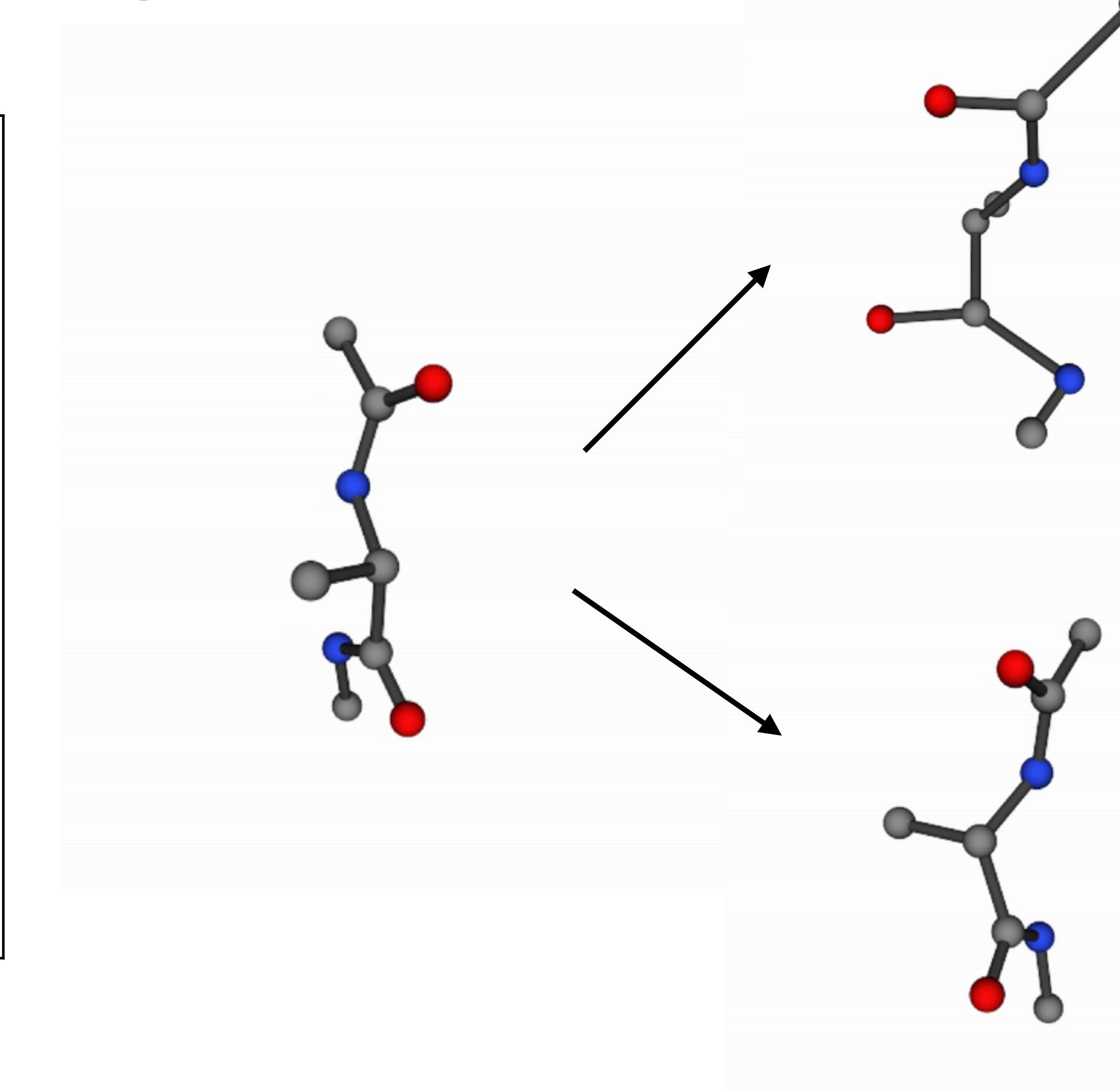
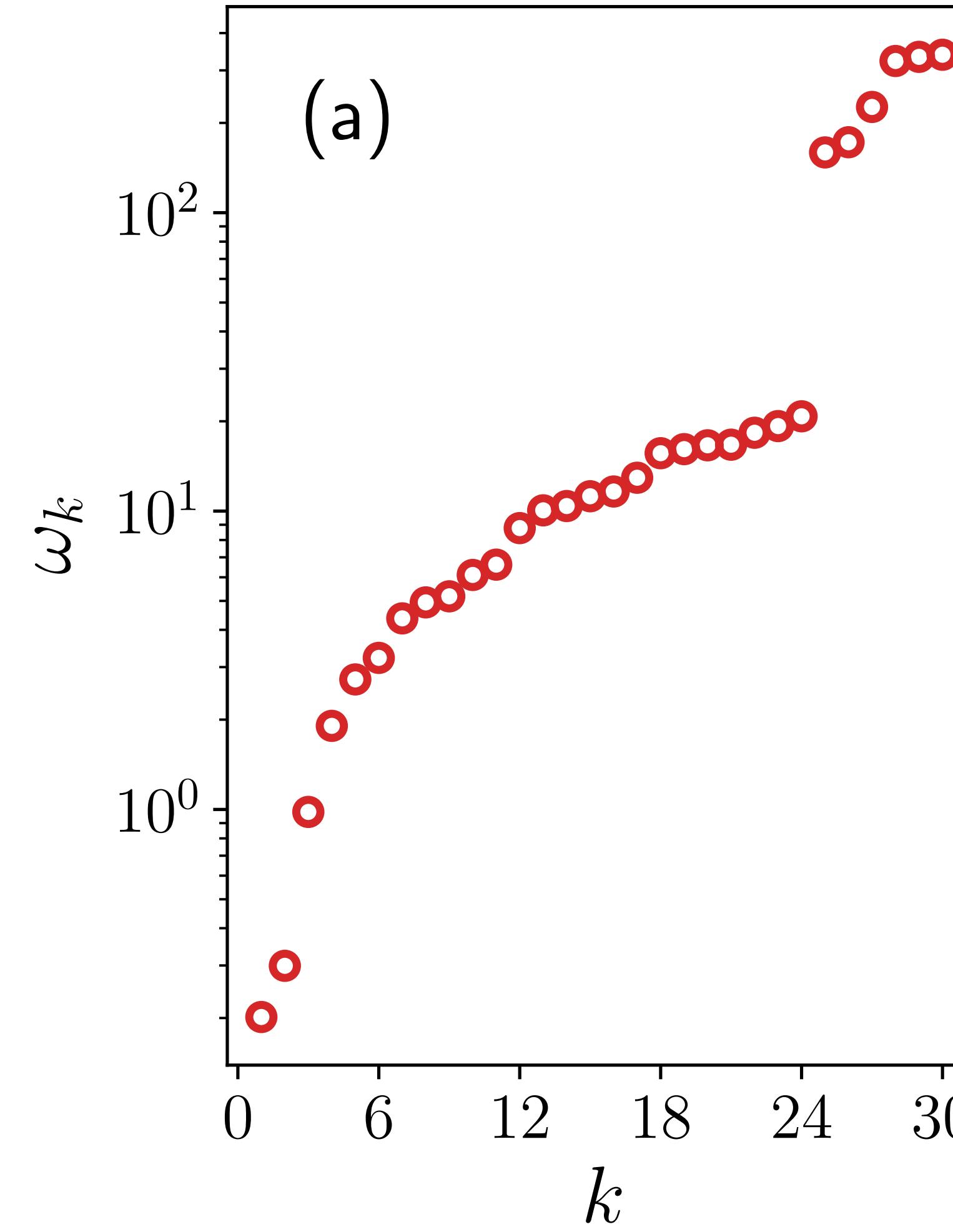


latent space

$$K(P, Q) = \sum_k \frac{P_k^2 + \omega_k^2 Q_k^2}{2}$$

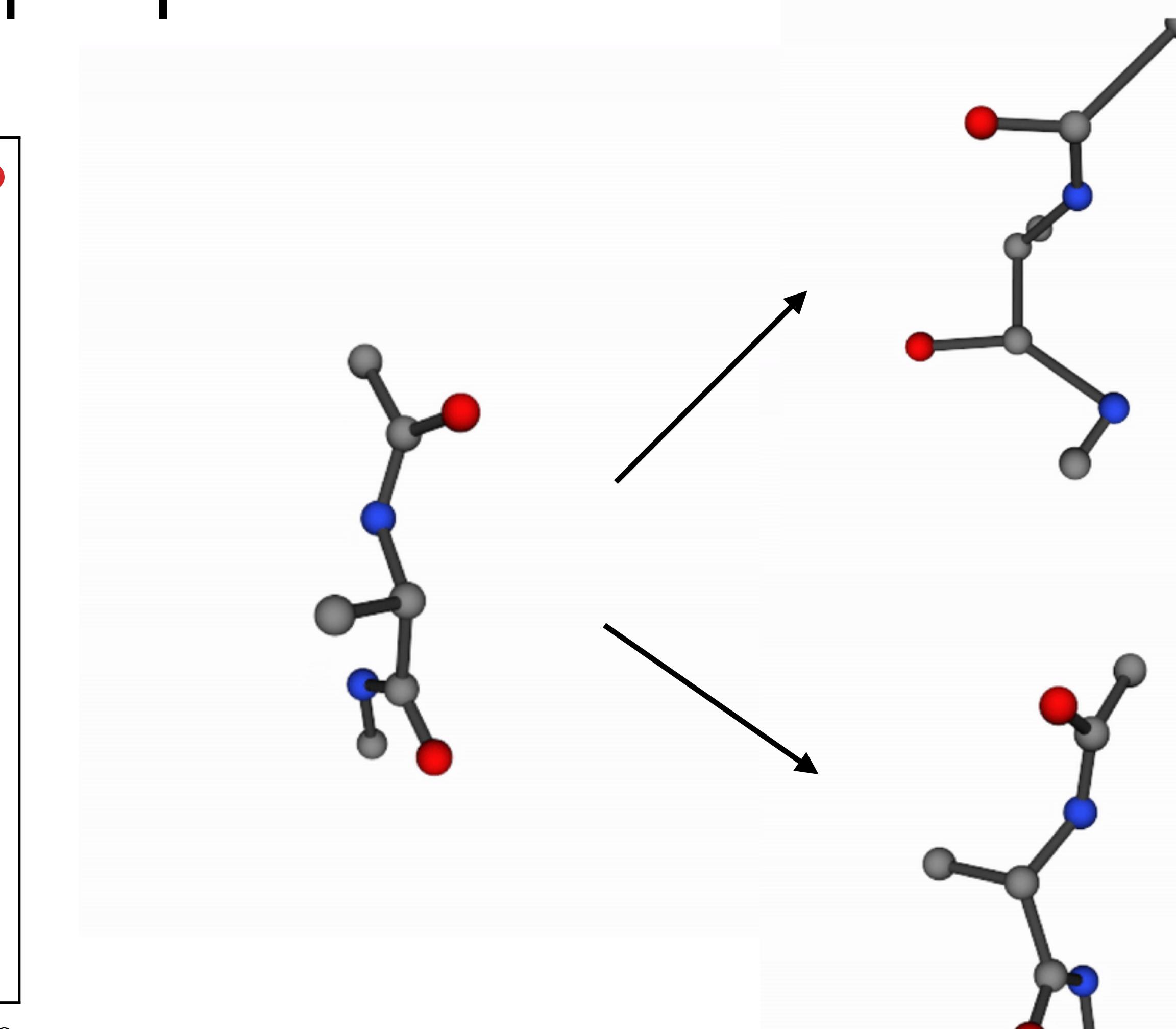
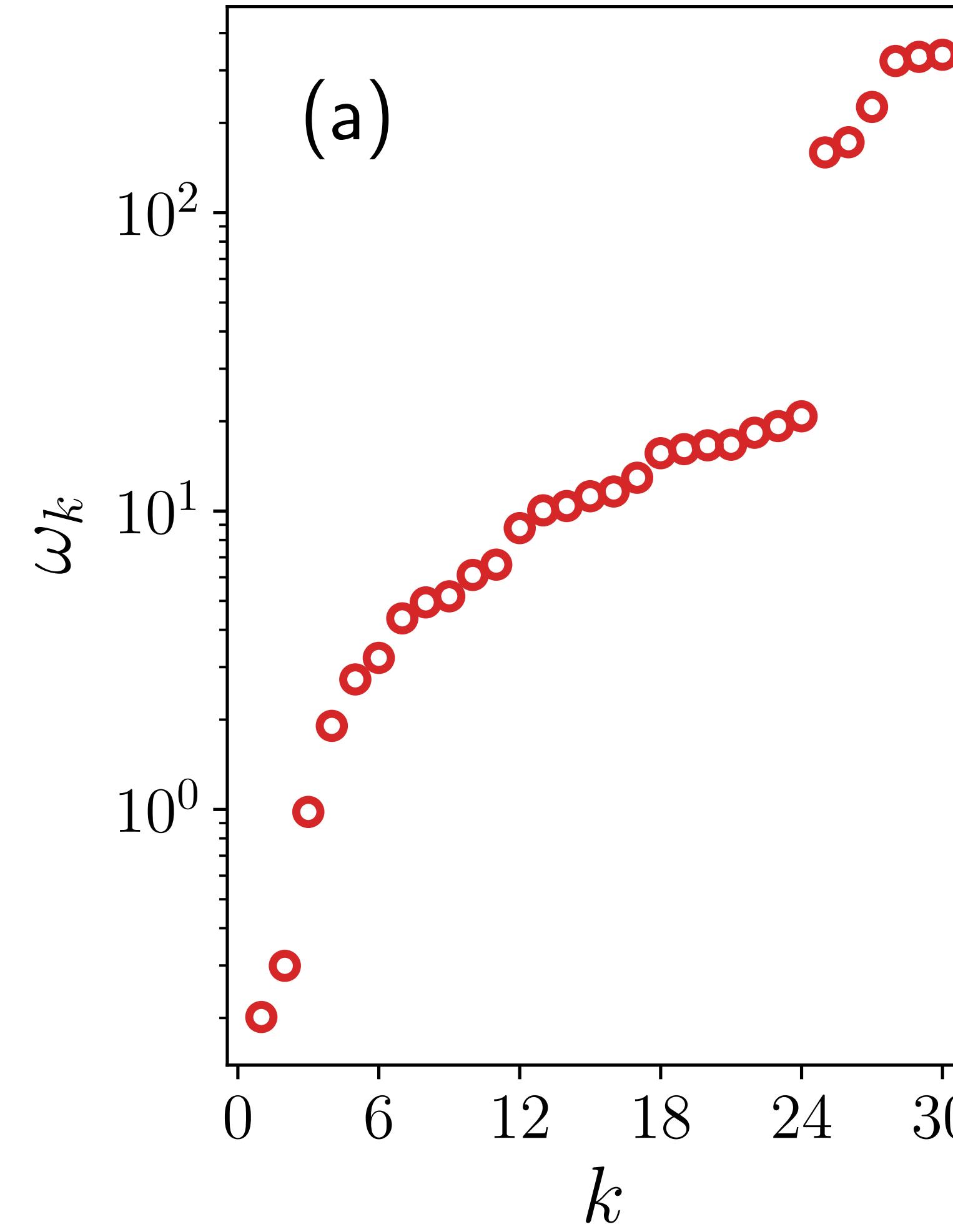
Learn the network parameter and the latent harmonic frequency

# Alanine dipeptide slow modes

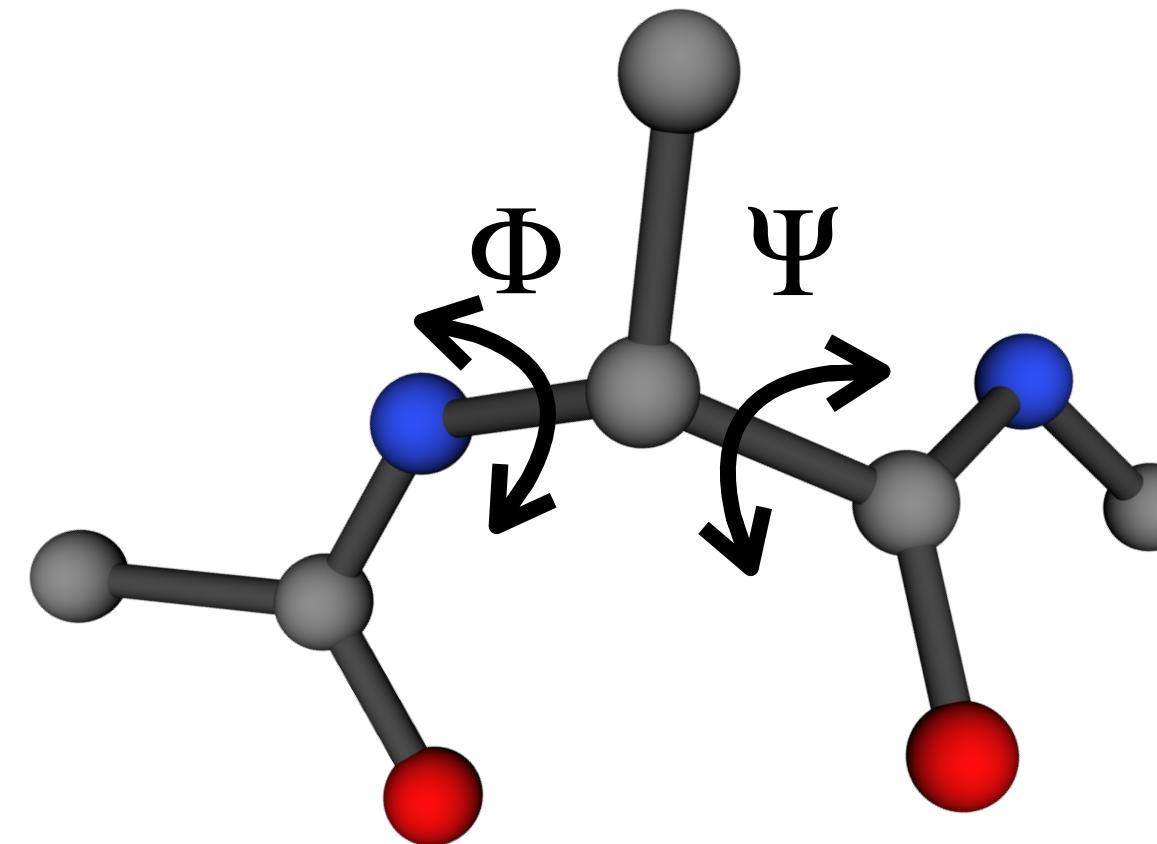


Neural canonical transformation identifies nonlinear slow modes!

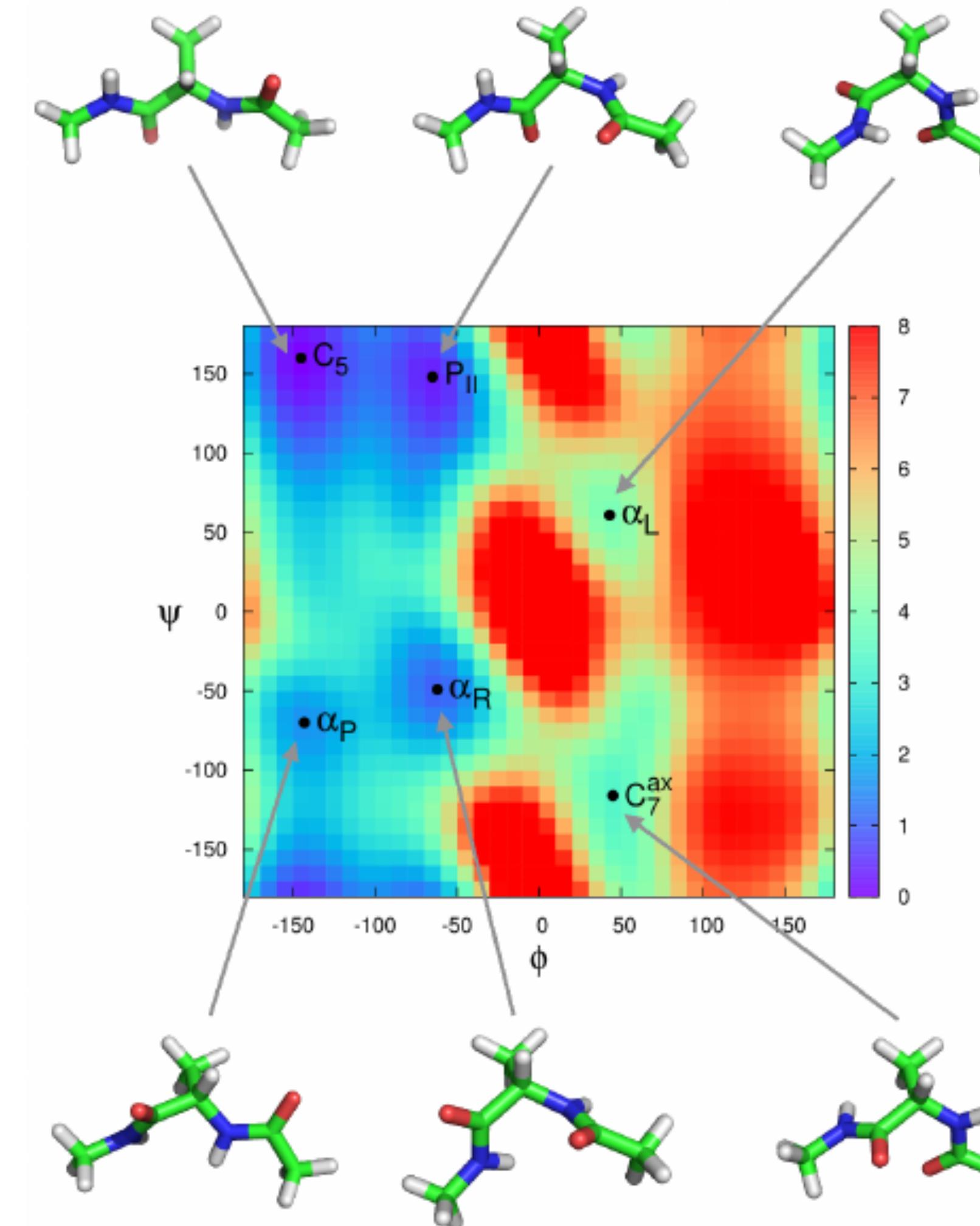
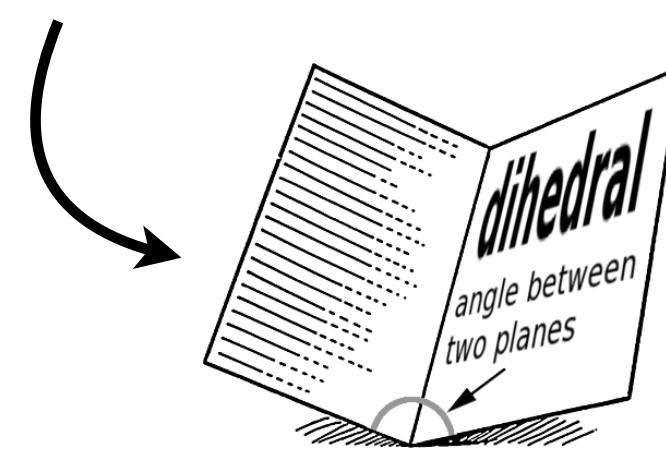
# Alanine dipeptide slow modes



Neural canonical transformation identifies nonlinear slow modes!



slow motion of the  
two torsion angles



Ramachandran  
plot of stable  
conformations

**Dimensional reduction to slow collective variables  
useful for control, prediction, enhanced sampling...**

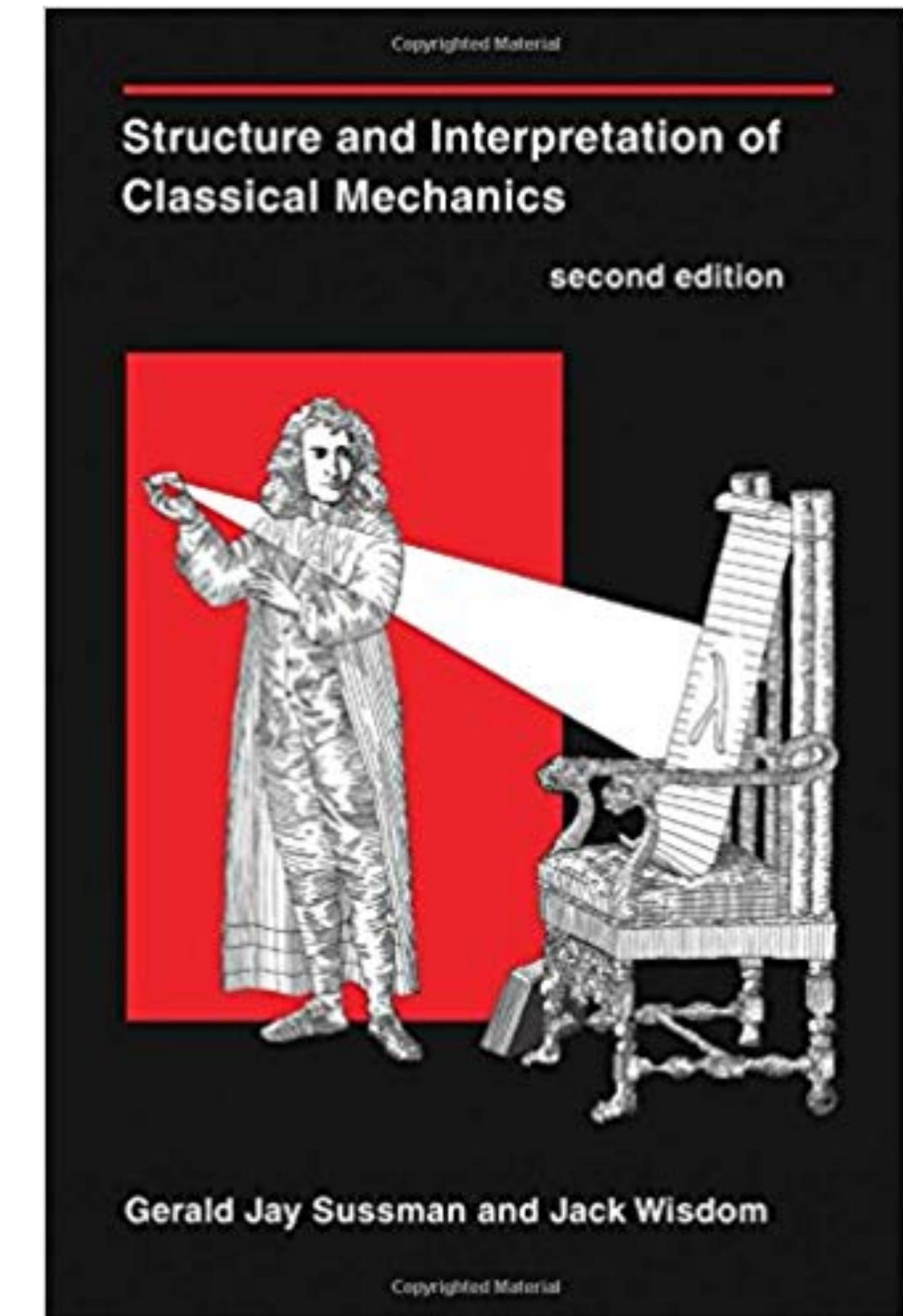
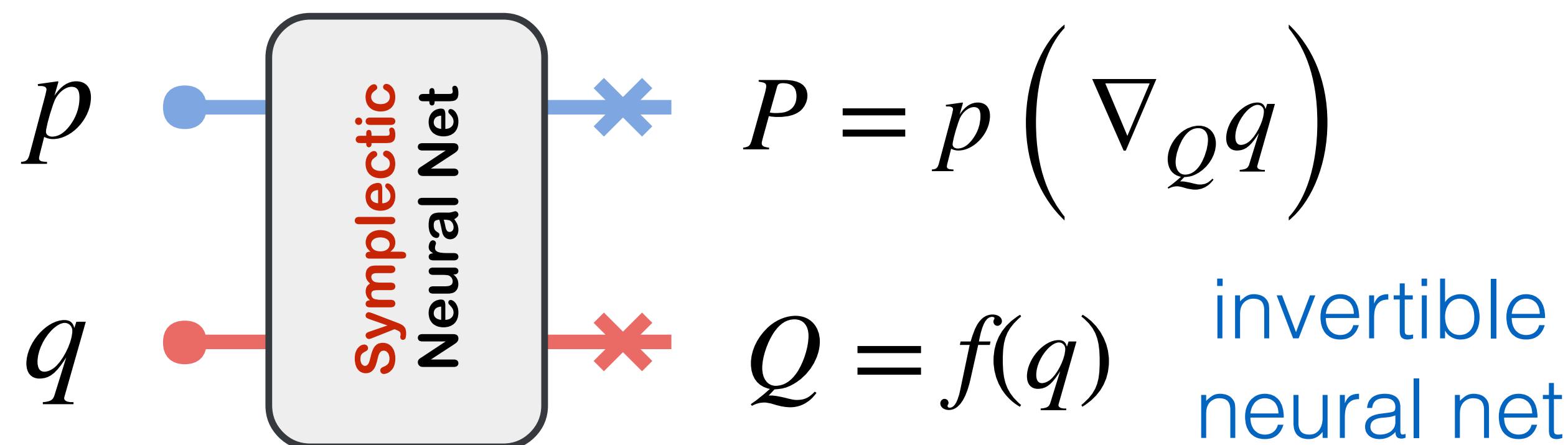
check the paper 1910.00024, PRX '20 for more examples & applications

# Symplectic primitives

- Linear transformation: Symplectic Lie algebra
- Continuous-time flow: Symplectic generating functions

Symplectic integrator of neural ODE, Chen et al 1806.07366

- **Neural point transformation**



# “A Hamiltonian Extravaganza”

—Danilo J. Rezende@DeepMind

Sep 25 **ICLR 2020 paper submission deadline**

Sep 26 *Symplectic ODE-Net*, 1909.12077  **SIEMENS**

Sep 27 *Hamiltonian Graph Networks with ODE Integrators*, 1909.12790 

Sep 29 *Symplectic RNN*, 1909.13334   

Sep 30 *Equivariant Hamiltonian Flows*, 1909.13739 

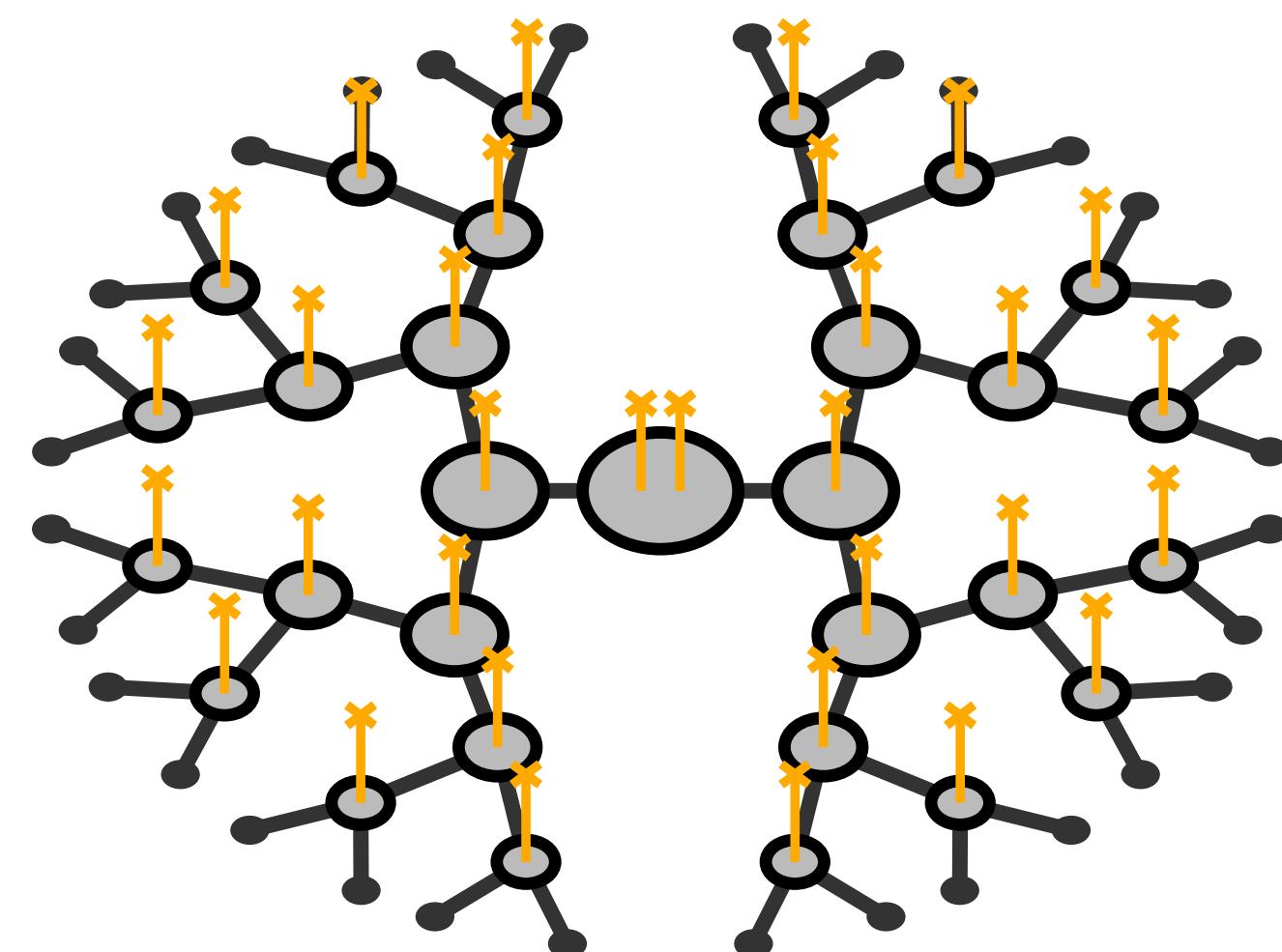
*Hamiltonian Generative Network*, 1909.13789  <http://tiny.cc/hgn>

*Neural Canonical Transformation with Symplectic Flows*, 1910.00024  

See also Bondesan & Lamacraft, *Learning Symmetries of Classical Integrable Systems*, 1906.04645

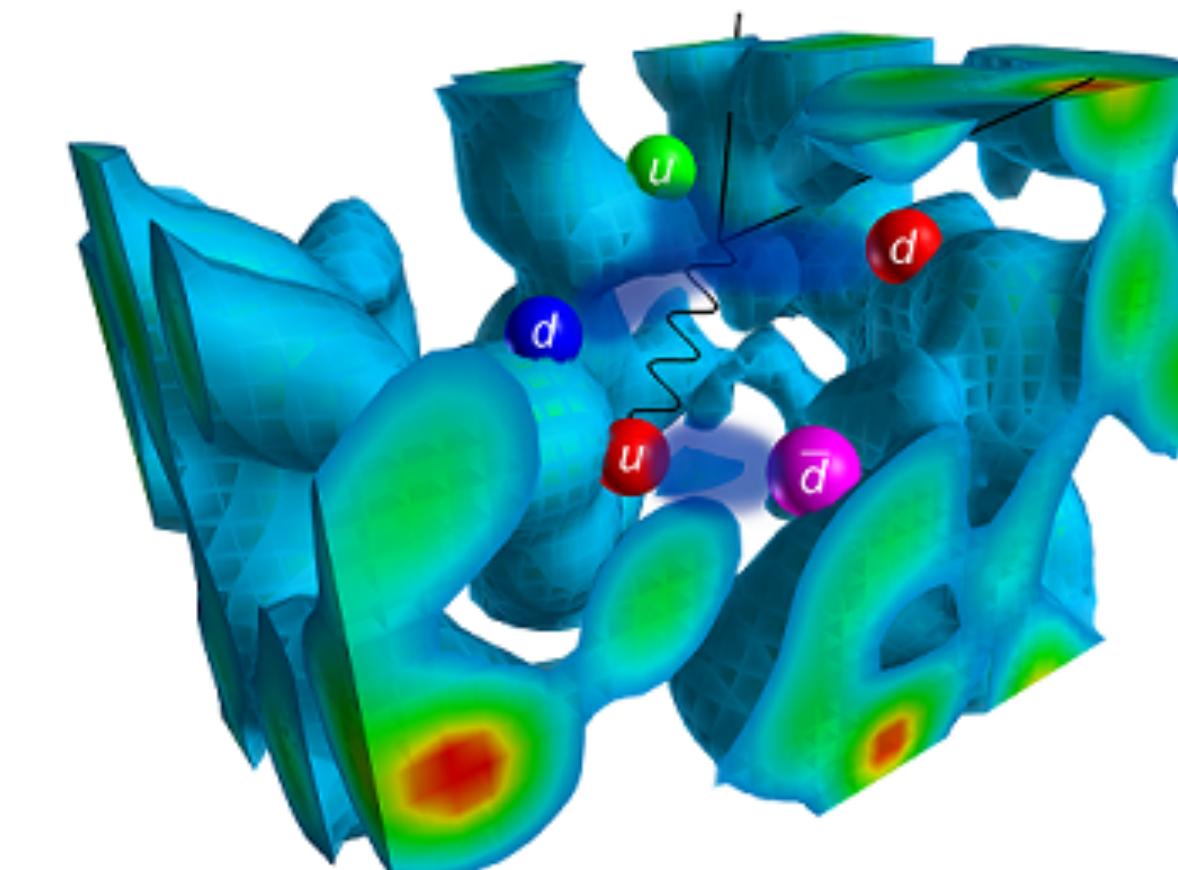
# Killer application in science ?

## Renormalization group



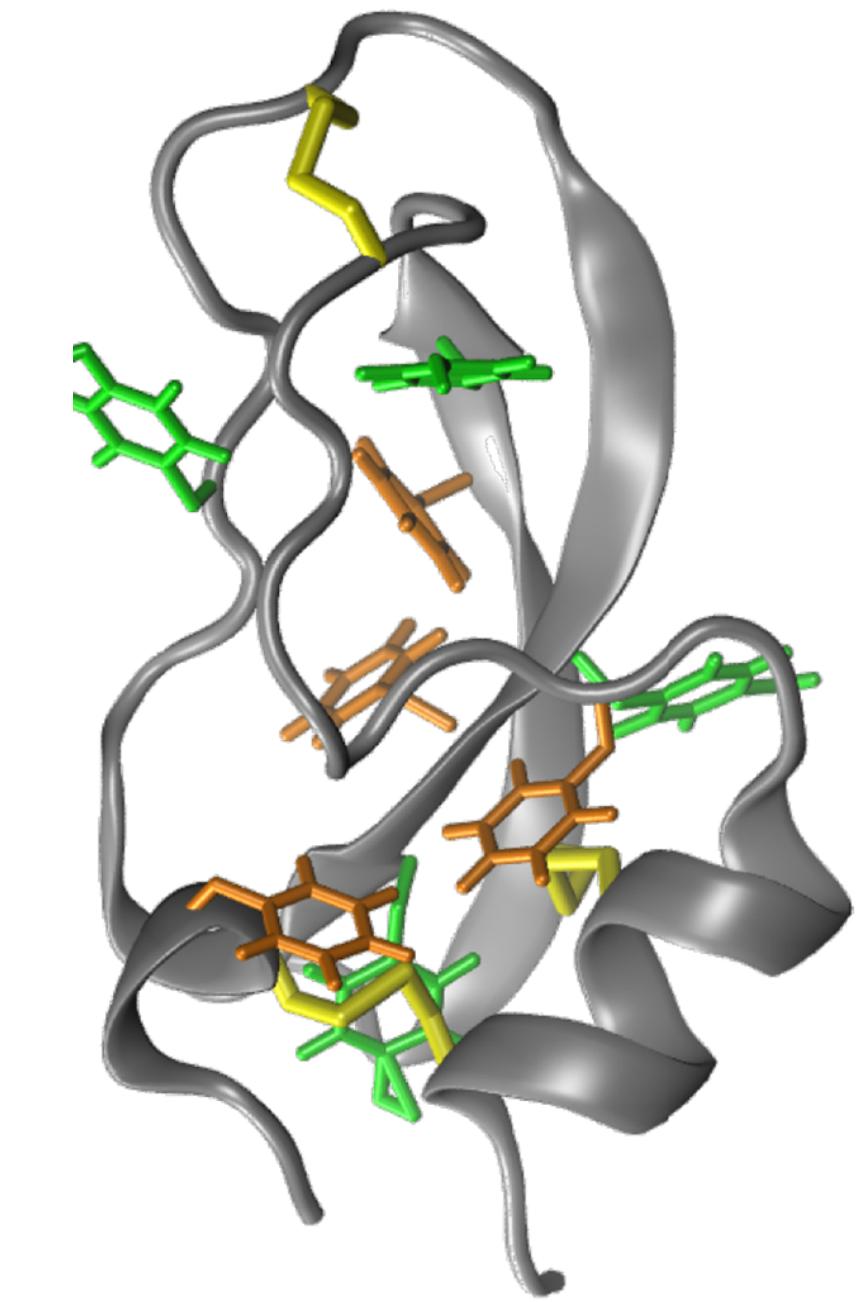
Li and LW, PRL '18  
Hu et al, PRResearch '20

## Lattice field theory



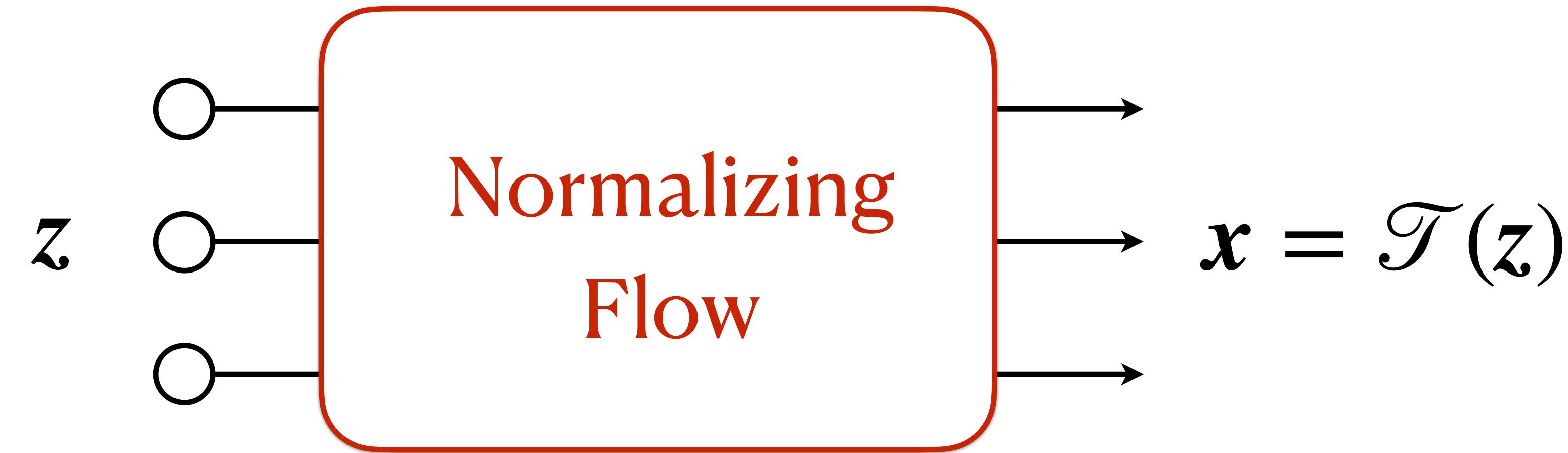
Albergo et al, PRD '19  
Kanwar et al, PRL '20

## Molecular simulation



Noe et al, Science '19  
Wirnsberger et al, JCP '20

# Symmetries



Invariance

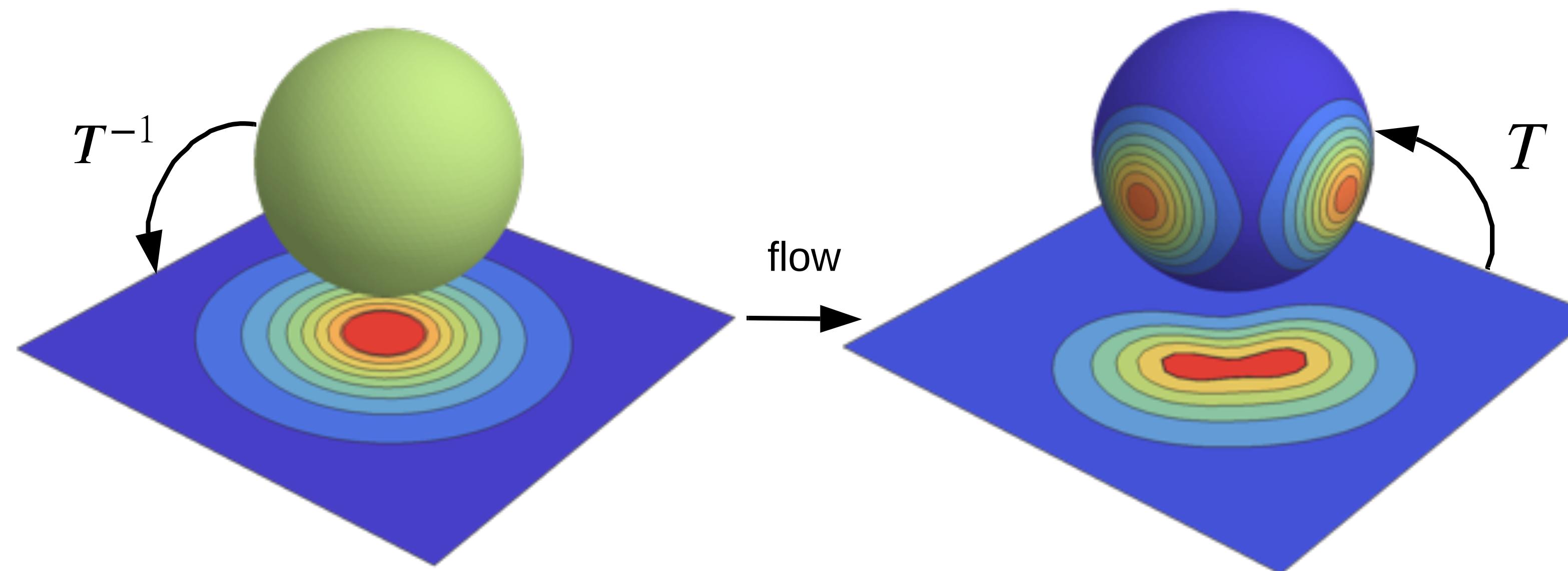
$$\rho(gx) = \rho(x)$$

Equivariance

$$\mathcal{T}(gz) = g\mathcal{T}(z)$$

Spatial symmetries, permutation symmetries, gauge symmetries...

# Flow on manifolds

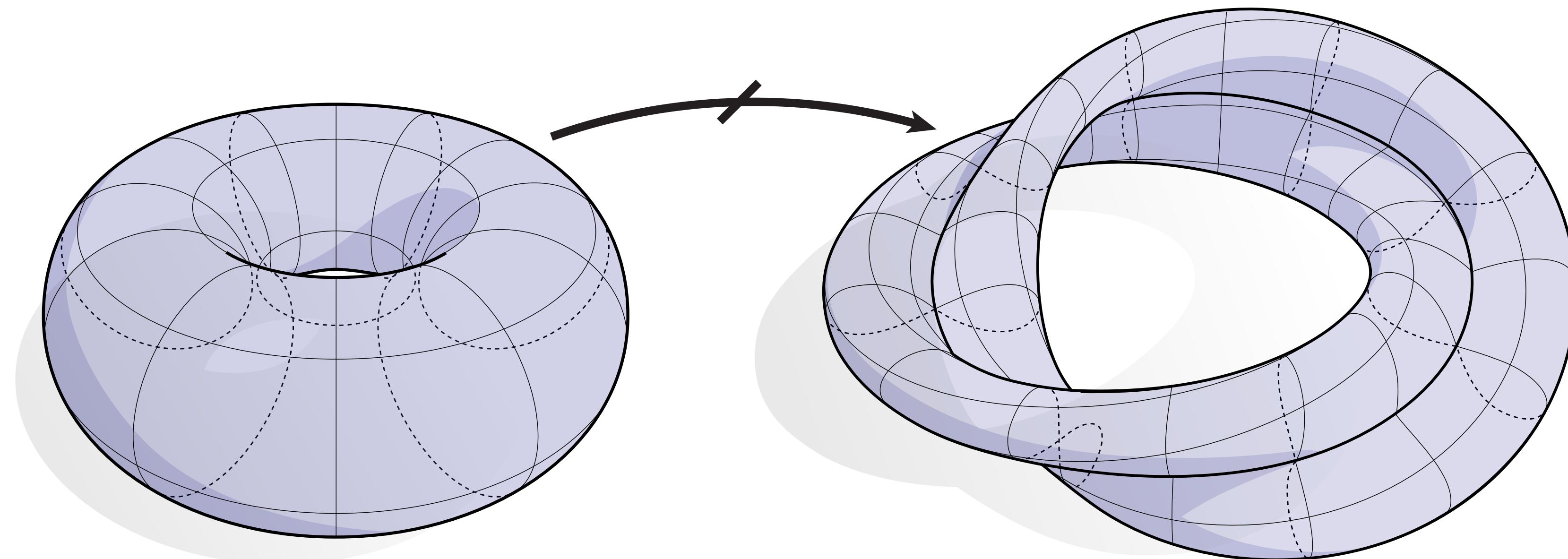


Periodic variables, gauge fields, ...

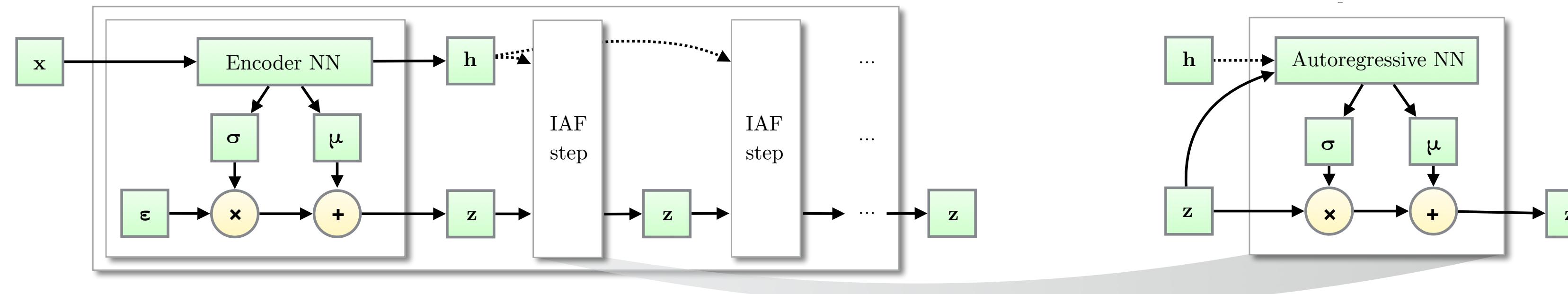
Gemici et al 1611.02304, Rezende et al, 2002.02428, Boyda et al, 2008.05456

Neural ODE on manifolds, Falorsi et al, 2006.06663, Lou et al, 2006.10254, Mathieu et al, 2006.10605

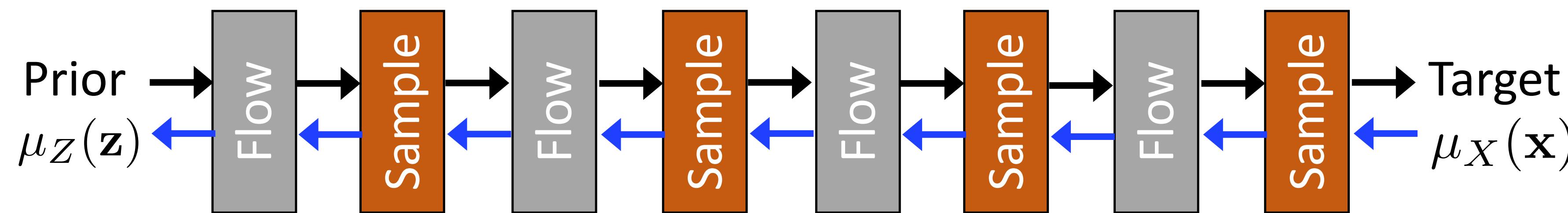
# Obstructions



# Mix with other approaches



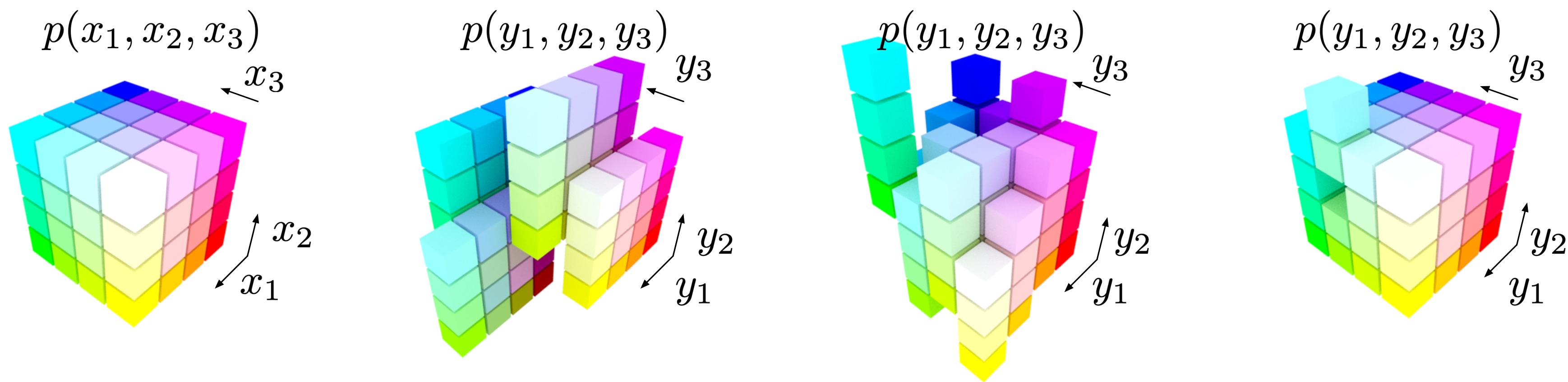
Kingma et al, 1606.04934, ...



Levy et al, 1711.09268, Wu et al 2002.06707, ...

# Discrete flows

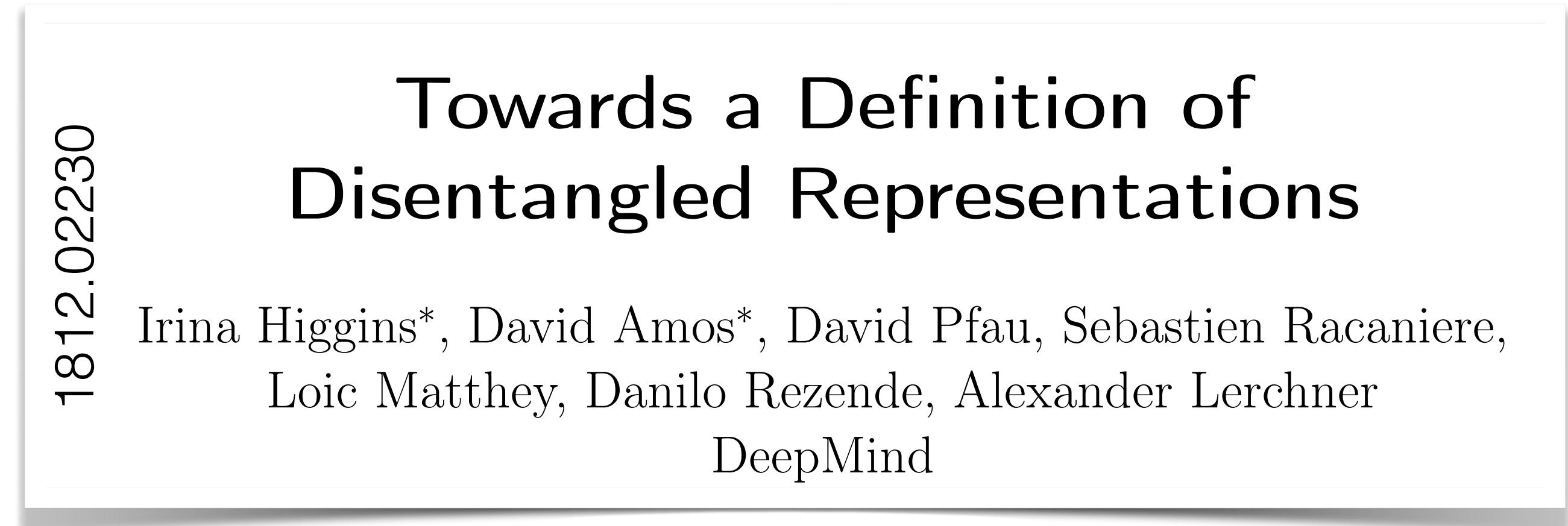
$$p(\mathbf{x}) = p(\mathbf{y} = \mathcal{T}(\mathbf{x}))$$



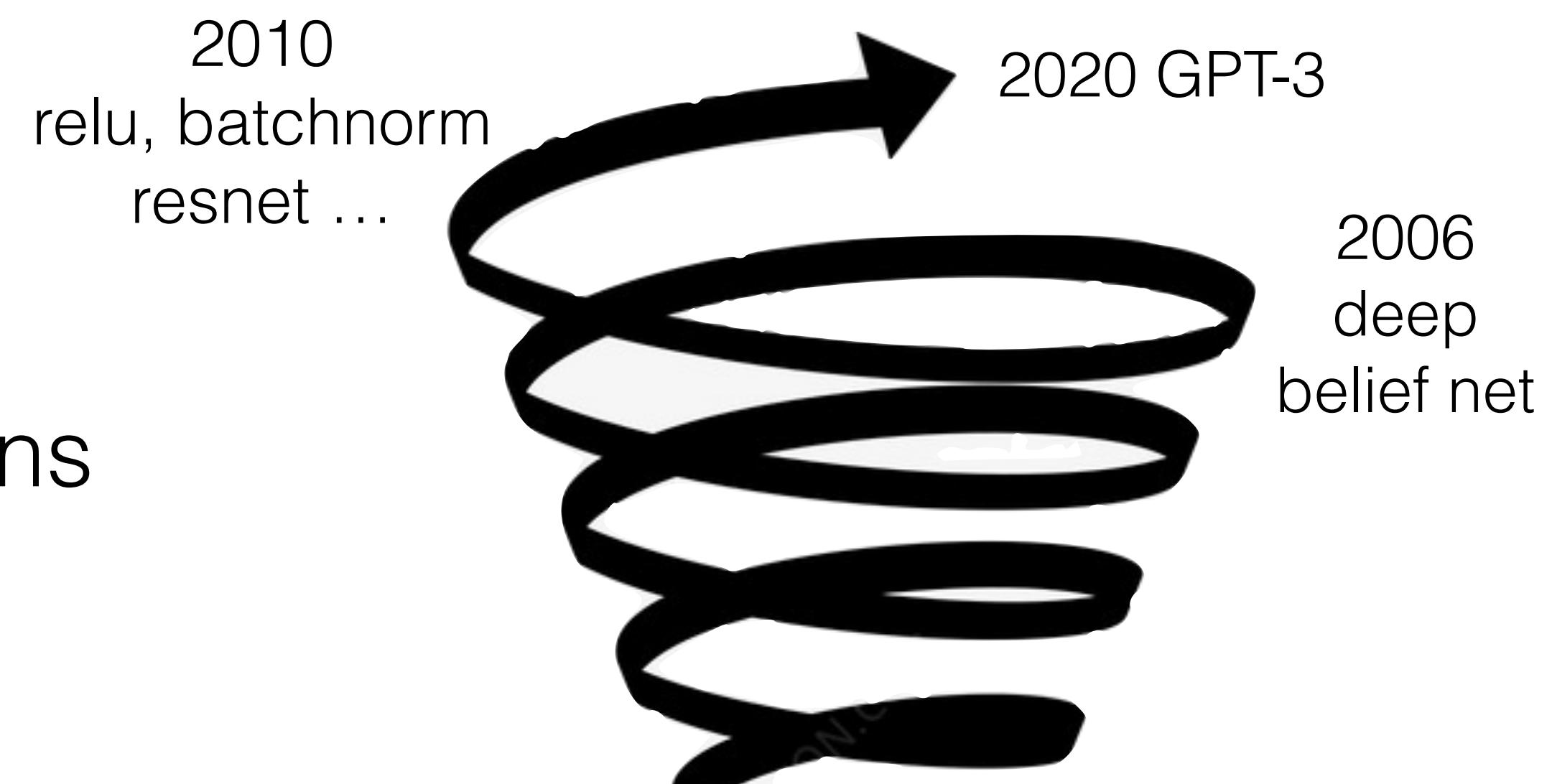
Tran et al, 1905.10347, Hoogeboom et al, 1905.07376, van den Berg 2006.12459

# Representation learning: what and how ?

What is a good representation ?



**Generative Pre-Training** appears to be a successful way in learning good representations



# Thank You!

Explore more in the interface  
of machine learning & physics

## 量子纠缠：从量子物质态到深度学习

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(1 中国科学院物理研究所 北京 100190)

(2 中国科学院大学 北京 100049)

《物理》2017年7月

## 微分万物：深度学习的启示\*

王 磊<sup>1,2,†</sup> 刘金国<sup>3</sup>

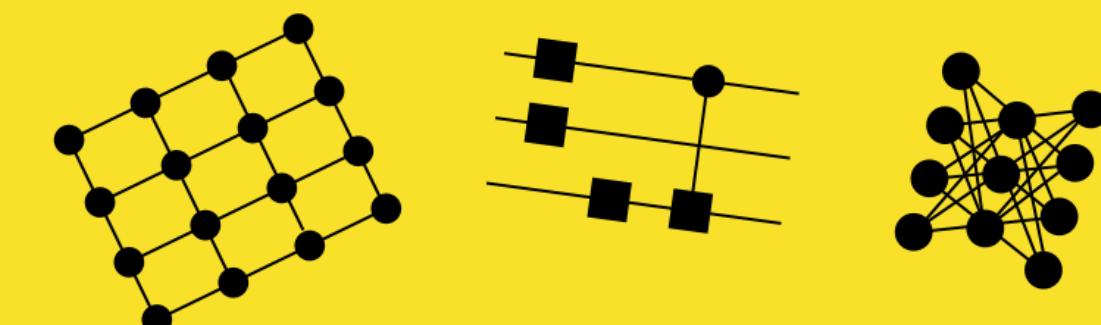
(1 中国科学院物理研究所 北京 100190)

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(3 哈佛大学物理系 剑桥 02138)

《物理》2021年2月

# Spring School



王磊

### 深度学习：从理论到实践

以微分编程和表示学习为重点  
介绍深度学习技术，并讲解它们在  
统计物理和量子多体计算中的应用实例

张潘

### 从机器学习角度理解张量网络

从表述，优化，学习与泛化这  
四个角度介绍张量网络及其  
在应用数学和机器学习中的应用

罗秀哲

### 面向物理学家的Julia编程实践

以量子物理的工程实践为重点介绍  
Julia语言，量子计算的基础概念，Julia  
语言中的CUDA编程和量子物理工具链

刘金国

### 量子编程实践

介绍量子机器学习，量子优化算法和  
量子化学中的研究前沿，基于Julia量子  
计算库Yao.jl实现这些算法，介绍自动  
微分与GPU编程在量子编程中的应用

报名方式：



[https://bit.ly/  
2CE5J8H](https://bit.ly/2CE5J8H)

教学资料：

[https://github.com/  
QuantumBFS/SSSS](https://github.com/QuantumBFS/SSSS)

授课形式：

中文授课+程序演示+Hackathon (有奖品)

时间：2019年5月6-10日

地点：广东东莞

松山湖材料实验室

粤港澳交叉科学中心

Quantum Hackathon：

学员将通过组队的形式，完成  
一个量子物理相关的编程挑战。  
我们将评出表现突出的团队，  
给予奖励。

Contact: [wanglei@iphy.ac.cn](mailto:wanglei@iphy.ac.cn)



QuantumBFS  
Yao Framework



SONGSHAN LAKE  
MATERIALS LABORATORY  
松山湖材料实验室